9-ANTHRACENECARBOXYLIC ACID

Other names:	9-anthroic acid
	9-carboxyanthracene
	ANCA
	Anthracene-10-carboxylic acid
	Anthracene-9-carboxylic acid
Inchi:	InChI=1S/C15H10O2/c16-15(17)14-12-7-3-1-5-10(12)9-11-6-2-4-8-13(11)14/h1-9H,(H,16
InchiKey:	XGWFJBFNAQHLEF-UHFFFAOYSA-N
Formula:	C15H10O2
SMILES:	O=C(O)c1c2ccccc2cc2ccccc12
Mol. weight [g/mol]:	222.24

Physical Properties

Property code	Value	Unit	Source
af	0.7694		Cheméo Relay (1.0)
gf	116.13	kJ/mol	Joback Method
hf	-152.94	kJ/mol	Cheméo Relay (1.0)
hfus	27.59	kJ/mol	Joback Method
hvap	104.19	kJ/mol	Cheméo Relay (1.0)
ie	7.51	eV	Cheméo Relay (1.0)
log10ws	-3.88		Cheméo Relay (1.0)
logp	3.691		Crippen Method
mcvol	166.970	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	663.00	K	Cheméo Relay (1.0)
tc	1006.78	K	Cheméo Relay (1.0)
tf	460.79	K	Cheméo Relay (1.0)
vc	0.598	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.96	J/mol×K	996.23	Joback Method
cpg	440.49	J/mol×K	763.25	Joback Method
cpg	450.84	J/mol×K	802.08	Joback Method

cpg	460.47	J/mol×K	840.91	Joback Method
cpg	469.49	J/mol×K	879.74	Joback Method
cpg	478.01	J/mol×K	918.57	Joback Method
cpg	486.13	J/mol×K	957.40	Joback Method
dvisc	0.0002967	Pa×s	624.84	Joback Method
dvisc	0.0001233	Pa×s	763.25	Joback Method
dvisc	0.0001591	Pa×s	717.11	Joback Method
dvisc	0.0002127	Pa×s	670.97	Joback Method
dvisc	0.0011761	Pa×s	486.42	Joback Method
dvisc	0.0004364	Pa×s	578.70	Joback Method
dvisc	0.0006863	Pa×s	532.56	Joback Method
hsubt	120.10 ± 3.80	kJ/mol	402.50	NIST Webbook
psub	4.47e-04	kPa	413.14	Thermodynamic study of 9-anthracenecarboxylic acid
psub	8.37e-04	kPa	419.14	Thermodynamic study of 9-anthracenecarboxylic acid
psub	3.12e-04	kPa	409.18	Thermodynamic study of 9-anthracenecarboxylic acid
psub	3.79e-04	kPa	411.14	Thermodynamic study of 9-anthracenecarboxylic acid
psub	3.78e-04	kPa	411.14	Thermodynamic study of 9-anthracenecarboxylic acid
psub	3.68e-04	kPa	411.14	Thermodynamic study of 9-anthracenecarboxylic acid
psub	4.70e-04	kPa	413.14	Thermodynamic study of 9-anthracenecarboxylic acid
psub	2.49e-04	kPa	407.14	Thermodynamic study of 9-anthracenecarboxylic acid
psub	4.44e-04	kPa	413.14	Thermodynamic study of 9-anthracenecarboxylic acid
psub	5.55e-04	kPa	415.19	Thermodynamic study of 9-anthracenecarboxylic acid

psub	5.76e-04	kPa	415.19	Thermodynamic study of 9-anthracenecarboxylic acid
psub	5.50e-04	kPa	415.19	Thermodynamic study of 9-anthracenecarboxylic acid
psub	6.78e-04	kPa	417.15	Thermodynamic study of 9-anthracenecarboxylic acid
psub	6.68e-04	kPa	417.15	Thermodynamic study of 9-anthracenecarboxylic acid
psub	6.48e-04	kPa	417.15	Thermodynamic study of 9-anthracenecarboxylic acid
psub	3.21e-04	kPa	409.18	Thermodynamic study of 9-anthracenecarboxylic acid
psub	8.16e-04	kPa	419.14	Thermodynamic study of 9-anthracenecarboxylic acid
psub	8.20e-04	kPa	419.14	Thermodynamic study of 9-anthracenecarboxylic acid
psub	1.00e-03	kPa	421.19	Thermodynamic study of 9-anthracenecarboxylic acid
psub	9.97e-04	kPa	421.19	Thermodynamic study of 9-anthracenecarboxylic acid
psub	9.97e-04	kPa	421.19	Thermodynamic study of 9-anthracenecarboxylic acid
psub	1.19e-03	kPa	423.12	Thermodynamic study of 9-anthracenecarboxylic acid
psub	1.18e-03	kPa	423.12	Thermodynamic study of 9-anthracenecarboxylic acid
psub	1.15e-03	kPa	423.12	Thermodynamic study of 9-anthracenecarboxylic acid
psub	2.55e-04	kPa	407.14	Thermodynamic study of 9-anthracenecarboxylic acid

psub	2.72e-04	kPa	407.14	Thermodynamic study of 9-anthracenecarboxylic acid
psub	2.12e-04	kPa	405.12	Thermodynamic study of 9-anthracenecarboxylic acid
psub	2.15e-04	kPa	405.12	Thermodynamic study of 9-anthracenecarboxylic acid
psub	2.18e-04	kPa	405.12	Thermodynamic study of 9-anthracenecarboxylic acid
psub	1.75e-04	kPa	403.16	Thermodynamic study of 9-anthracenecarboxylic acid
psub	1.80e-04	kPa	403.16	Thermodynamic study of 9-anthracenecarboxylic acid
psub	1.80e-04	kPa	403.16	Thermodynamic study of 9-anthracenecarboxylic acid

Sources

Cheméo Relay (1.0, beta):

Thermodynamic study of 9-anthracenecarboxylic acid: https://www.doi.org/10.1016/j.jct.2010.08.018

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C723626&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume