

2-Anthracenecarboxylic acid

Other names:	2-Anthroic acid Anthracene-2-carboxylic acid
Inchi:	InChI=1S/C15H10O2/c16-15(17)13-6-5-12-7-10-3-1-2-4-11(10)8-14(12)9-13/h1-9H,(H,16)
InchiKey:	RZRJYURCNBXIST-UHFFFAOYSA-N
Formula:	C15H10O2
SMILES:	O=C(O)c1ccc2cc3ccccc3cc2c1
Mol. weight [g/mol]:	222.24
CAS:	613-08-1

Physical Properties

Property code	Value	Unit	Source
gf	116.13	kJ/mol	Joback Method
hf	-22.01	kJ/mol	Joback Method
hfus	27.59	kJ/mol	Joback Method
hvap	79.29	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	3.691		Crippen Method
mvol	166.970	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	763.25	K	Joback Method
tc	996.23	K	Joback Method
tf	486.42	K	Joback Method
vc	0.636	m ³ /kmol	Joback Method

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	0.0001233	Paxs	763.25	Joback Method
dvisc	0.0011761	Paxs	486.42	Joback Method
dvisc	0.0006863	Paxs	532.56	Joback Method
dvisc	0.0004364	Paxs	578.70	Joback Method
dvisc	0.0002967	Paxs	624.84	Joback Method
dvisc	0.0002127	Paxs	670.97	Joback Method
dvisc	0.0001591	Paxs	717.11	Joback Method
hsubt	134.80 ± 3.40	kJ/mol	411.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C613081&Units=SI

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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