10-Methylanthracene-9-carboxaldehyde

Other names:	9-Anthracenecarboxaldehyde, 10-methyl- 10-methylanthracene-9-carbaldehyde
Inchi:	InChI=1S/C16H12O/c1-11-12-6-2-4-8-14(12)16(10-17)15-9-5-3-7-13(11)15/h2-10H,1H3
InchiKey:	KVWSVUPNZVIFBN-UHFFFAOYSA-N
Formula:	C16H12O
SMILES:	Cc1c2ccccc2c(C=O)c2ccccc12
Mol. weight [g/mol]:	220.27
CAS:	7072-00-6

Physical Properties

Property code	Value	Unit	Source
gf	281.14	kJ/mol	Joback Method
hf	125.11	kJ/mol	Joback Method
hfus	26.40	kJ/mol	Joback Method
hvap	65.47	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.114		Crippen Method
mcvol	175.190	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	383.10		NIST Webbook
tb	693.72	K	Joback Method
tc	938.84	K	Joback Method
tf	441.46	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.54	J/mol×K	693.72	Joback Method
cpg	503.09	J/mol×K	897.99	Joback Method
cpg	492.93	J/mol×K	857.14	Joback Method
cpg	482.12	J/mol×K	816.28	Joback Method
cpg	470.53	J/mol×K	775.43	Joback Method
cpg	458.04	J/mol×K	734.57	Joback Method

cpg	512.70	J/mol×K	938.84	Joback Method
dvisc	0.0005434	Pa×s	693.72	Joback Method
dvisc	0.0006129	Pa×s	651.68	Joback Method
dvisc	0.0007029	Pa×s	609.63	Joback Method
dvisc	0.0008226	Pa×s	567.59	Joback Method
dvisc	0.0009872	Pa×s	525.55	Joback Method
dvisc	0.0012229	Pa×s	483.50	Joback Method
dvisc	0.0015780	Pa×s	441.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7072006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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