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

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

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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