1,2,3,4-Tetrahydrochrysene

Other names: Chrysene, 1,2,3,4-tetrahydro-
1,2,3,4-tetrahydrocrysene
Inchi: InChI=1S/C18H16/c1-3-7-15-13(5-1)9-11-18-16-8-4-2-6-14(16)10-12-17(15)18/h1,3,5,7,9
InchiKey: YMLBMIKSAYQNNI-UHFFFAOYSA-N
Formula: C18H16
SMILES: c1ccc2c(c1)ccc1c3c(ccc12)CCCC3
Mol. weight [g/mol]: 232.32
CAS: 2091-90-9

Physical Properties

Property code	Value	Unit	Source
gf	453.86	kJ/mol	Joback Method
hf	256.39	kJ/mol	Joback Method
hfus	24.25	kJ/mol	Joback Method
hvap	63.60	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	4.872		Crippen Method
mcvol	190.940	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	2213.00		NIST Webbook
tb	706.50	K	Joback Method
tc	965.08	K	Joback Method
tf	440.66	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.50	J/mol×K	706.50	Joback Method
cpg	533.70	J/mol×K	749.60	Joback Method
cpg	549.56	J/mol×K	792.69	Joback Method
cpg	564.30	J/mol×K	835.79	Joback Method
cpg	578.10	J/mol×K	878.88	Joback Method
cpg	591.17	J/mol×K	921.98	Joback Method

cpg	603.71	J/mol×K	965.08	Joback Method
dvisc	0.0018601	Pa×s	440.66	Joback Method
dvisc	0.0014399	Pa×s	484.97	Joback Method
dvisc	0.0011635	Pa×s	529.27	Joback Method
dvisc	0.0009716	Pa×s	573.58	Joback Method
dvisc	0.0008326	Pa×s	617.89	Joback Method
dvisc	0.0007283	Pa×s	662.19	Joback Method
dvisc	0.0006479	Pa×s	706.50	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2091909&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
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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