Chrysene, 1,2,3,4,4a,7,8,9,10,11,12,12a-dodecahydro-

Other names: 1,2,3,4,4a,7,8,9,10,11,12,12a-Dodecahydrochrysene
1,2,3,4,5,6,6a,7,8,9,10,10a-Dodecahydrochrysene
NSC 114857
1,2,3,4,4A,7,8,9,10,12,12a-dodecahydrochrysene

Inchi: InChI=1S/C18H24/c1-3-7-15-13(5-1)9-11-18-16-8-4-2-6-14(16)10-12-17(15)18/h9,11,14,

InchiKey: DISXLARWFONJQP-UHFFFAOYSA-N

Formula: C18H24

SMILES: c1cc2c(c3c1CCCC3)CCC1CCCCC21

Mol. weight [g/mol]: 240.38

CAS: 1610-22-6

Physical Properties

Property code	Value	Unit	Source
gf	337.86	kJ/mol	Joback Method
hf	7.53	kJ/mol	Joback Method
hfus	22.28	kJ/mol	Joback Method
hvap	60.49	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.785		Crippen Method
mcvol	208.140	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
tb	690.56	K	Joback Method
tc	938.43	K	Joback Method
tf	404.10	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.46	J/mol×K	897.12	Joback Method
cpg	702.18	J/mol×K	855.81	Joback Method
cpg	683.67	J/mol×K	814.50	Joback Method
cpg	663.77	J/mol×K	773.18	Joback Method
cpg	642.30	J/mol×K	731.87	Joback Method

cpg	619.11	J/mol×K	690.56	Joback Method
cpg	735.67	J/mol×K	938.43	Joback Method
dvisc	0.0026806	Pa×s	404.10	Joback Method
dvisc	0.0007621	Pa×s	690.56	Joback Method
dvisc	0.0008694	Pa×s	642.82	Joback Method
dvisc	0.0010131	Pa×s	595.07	Joback Method
dvisc	0.0012124	Pa×s	547.33	Joback Method
dvisc	0.0015016	Pa×s	499.59	Joback Method
dvisc	0.0019458	Pa×s	451.84	Joback Method
hsubt	115.40	kJ/mol	303.00	NIST Webbook
hvapt	84.20	kJ/mol	338.00	NIST Webbook

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=C1610226&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
hvapt: Enthalpy of vaporization at a given temperature
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