Chrysene-D12

Other names: Chrysene - d
Chrysene, perdeutero-
Inchi: InChI=1S/C18H12/c1-3-7-15-13(5-1)9-11-18-16-8-4-2-6-14(16)10-12-17(15)18/h1-12H/i1
InchiKey: WDECIBYCCFPHNR-AQZSQYOVSA-N
Formula: C18D12
SMILES: c1ccc2c(c1)ccc1c3ccccc3ccc21
Mol. weight [g/mol]: 240.36
CAS: 1719-03-5

Physical Properties

Property code	Value	Unit	Source
gf	513.78	kJ/mol	Joback Method
hf	371.95	kJ/mol	Joback Method
hfus	26.70	kJ/mol	Joback Method
hvap	106.00	kJ/mol	NIST Webbook
log10ws	-6.88		Crippen Method
logp	5.146		Crippen Method
mcvol	182.340	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
tb	704.82	K	Joback Method
tc	968.39	K	Joback Method
tf	442.18	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.24	J/mol×K	968.39	Joback Method
cpg	532.31	J/mol×K	924.47	Joback Method
cpg	521.02	J/mol×K	880.54	Joback Method
cpg	509.15	J/mol×K	836.61	Joback Method
cpg	496.51	J/mol×K	792.68	Joback Method
cpg	482.86	J/mol×K	748.75	Joback Method
cpg	468.00	J/mol×K	704.82	Joback Method

dvisc	0.0017235	Pa×s	442.18	Joback Method
dvisc	0.0007153	Pa×s	704.82	Joback Method
dvisc	0.0007890	Pa×s	661.05	Joback Method
dvisc	0.0008825	Pa×s	617.27	Joback Method
dvisc	0.0010040	Pa×s	573.50	Joback Method
dvisc	0.0011669	Pa×s	529.73	Joback Method
dvisc	0.0013935	Pa×s	485.95	Joback Method
hvapt	106.04	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects:	https://www.doi.org/10.1021/je800091s
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=C1719035&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
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