

dibenzo[a,h]anthracene-d14

Inchi:	InChI=1S/C22H14/c1-3-7-19-15(5-1)9-11-17-14-22-18(13-21(17)19)12-10-16-6-2-4-8-20
InchiKey:	LHRCREOYAASXPZ-FPSGDROZSA-N
Formula:	C22H2D12
SMILES:	c1ccc2c(c1)ccc1cc3c(ccc4ccccc43)cc12
Mol. weight [g/mol]:	290.42

Physical Properties

Property code	Value	Unit	Source
gf	644.48	kJ/mol	Joback Method
hf	468.99	kJ/mol	Joback Method
hfus	33.69	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	6.299		Crippen Method
mcvol	219.240	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpola	494.21		NIST Webbook
tb	820.30	K	Joback Method
tc	1089.89	K	Joback Method
tf	532.48	K	Joback Method
vc	0.848	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.64	J/molxK	820.30	Joback Method
cpg	622.45	J/molxK	865.23	Joback Method
cpg	636.52	J/molxK	910.16	Joback Method
cpg	650.13	J/molxK	955.09	Joback Method
cpg	663.56	J/molxK	1000.03	Joback Method
cpg	677.10	J/molxK	1044.96	Joback Method
cpg	691.04	J/molxK	1089.89	Joback Method
dvisc	0.0022584	Paxs	532.48	Joback Method
dvisc	0.0019125	Paxs	580.45	Joback Method

dvisc	0.0016611	Paxs	628.42	Joback Method
dvisc	0.0014719	Paxs	676.39	Joback Method
dvisc	0.0013254	Paxs	724.36	Joback Method
dvisc	0.0012090	Paxs	772.33	Joback Method
dvisc	0.0011148	Paxs	820.30	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R394608&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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