

4,8-dibutylidene-2-thiaadamantane

Inchi: InChI=1S/C17H26S/c1-3-5-7-14-12-9-13-11-16(14)18-17(10-12)15(13)8-6-4-2/h7-8,12-14
InchiKey: OSTAESXMEDMFTD-IROCBMIISA-N
Formula: C17H26S
SMILES: CCCC=C1C2CC3CC1SC(C2)C3=CCCC
Mol. weight [g/mol]: 262.45

Physical Properties

Property code	Value	Unit	Source
gf	385.48	kJ/mol	Joback Method
hf	-4.99	kJ/mol	Joback Method
hfus	37.46	kJ/mol	Joback Method
hvap	60.42	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.353		Crippen Method
mcvol	225.560	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	1973.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2005.00		NIST Webbook
rinpol	1962.00		NIST Webbook
rinpol	2020.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1983.00		NIST Webbook
tb	669.29	K	Joback Method
tc	883.59	K	Joback Method
tf	431.58	K	Joback Method
vc	0.862	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.04	J/mol×K	669.29	Joback Method

cpg	668.58	J/mol×K	705.01	Joback Method
cpg	687.89	J/mol×K	740.72	Joback Method
cpg	706.09	J/mol×K	776.44	Joback Method
cpg	723.31	J/mol×K	812.16	Joback Method
cpg	739.66	J/mol×K	847.87	Joback Method
cpg	755.26	J/mol×K	883.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R207975&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

Legend

cpg:	Ideal gas heat capacity
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
mvol:	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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