

4,8-dibutyl-2-thiaadamantane

Inchi:	InChI=1S/C17H30S/c1-3-5-7-14-12-9-13-11-16(14)18-17(10-12)15(13)8-6-4-2/h12-17H,3
InchiKey:	URKLLDGPLCCAFC-UHFFFAOYSA-N
Formula:	C17H30S
SMILES:	CCCCC1C2CC3CC1SC(C2)C3CCCC
Mol. weight [g/mol]:	266.49

Physical Properties

Property code	Value	Unit	Source
gf	279.14	kJ/mol	Joback Method
hf	-197.73	kJ/mol	Joback Method
hfus	38.96	kJ/mol	Joback Method
hvap	58.23	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.513		Crippen Method
mcvol	234.160	ml/mol	McGowan Method
pc	1550.00	kPa	Joback Method
rinpol	2104.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2092.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2103.00		NIST Webbook
rinpol	2115.00		NIST Webbook
rinpol	2128.00		NIST Webbook
rinpol	2057.00		NIST Webbook
rinpol	2104.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2057.00		NIST Webbook
tb	646.67	K	Joback Method
tc	849.54	K	Joback Method
tf	402.38	K	Joback Method
vc	0.893	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.24	J/mol×K	646.67	Joback Method
cpg	717.50	J/mol×K	680.48	Joback Method
cpg	739.43	J/mol×K	714.29	Joback Method
cpg	760.11	J/mol×K	748.10	Joback Method
cpg	779.63	J/mol×K	781.91	Joback Method
cpg	798.08	J/mol×K	815.72	Joback Method
cpg	815.55	J/mol×K	849.54	Joback Method

Sources

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=R207960&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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