

4,8-dipropylidene-2-thiaadamantane

Inchi:	InChI=1S/C15H22S/c1-3-5-12-10-7-11-9-14(12)16-15(8-10)13(11)6-4-2/h5-6,10-11,14-15
InchiKey:	FNHNHDYEQKIOJM-BYDSPXIWSA-N
Formula:	C15H22S
SMILES:	CCC=C1C2CC3CC1SC(C2)C3=CCC
Mol. weight [g/mol]:	234.40

Physical Properties

Property code	Value	Unit	Source
gf	368.64	kJ/mol	Joback Method
hf	36.29	kJ/mol	Joback Method
hfus	32.28	kJ/mol	Joback Method
hvap	55.97	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.573		Crippen Method
mcvol	197.380	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1802.00		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	1799.00		NIST Webbook
rinpol	1814.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1817.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1839.00		NIST Webbook
rinpol	1787.00		NIST Webbook
tb	623.53	K	Joback Method
tc	845.33	K	Joback Method
tf	409.04	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.62	J/molxK	623.53	Joback Method

cpg	559.71	J/mol×K	660.50	Joback Method
cpg	578.50	J/mol×K	697.46	Joback Method
cpg	596.11	J/mol×K	734.43	Joback Method
cpg	612.65	J/mol×K	771.39	Joback Method
cpg	628.27	J/mol×K	808.36	Joback Method
cpg	643.09	J/mol×K	845.33	Joback Method

Sources

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=R208027&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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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