4,8-dipropyl-2-thiaadamantane

Inchi: InChI=1S/C15H26S/c1-3-5-12-10-7-11-9-14(12)16-15(8-10)13(11)6-4-2/h10-15H,3-9H2,1
InchiKey: ZJMZEHFJOGVBHY-UHFFFAOYSA-N
Formula: C15H26S
SMILES: CCCC1C2CC3CC1SC(C2)C3CCC
Mol. weight [g/mol]: 238.43

Physical Properties

Property code	Value	Unit	Source
gf	262.30	kJ/mol	Joback Method
hf	-156.45	kJ/mol	Joback Method
hfus	33.78	kJ/mol	Joback Method
hvap	53.78	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.733		Crippen Method
mcvol	205.980	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1906.00		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1889.00		NIST Webbook
rinpol	1918.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1882.00		NIST Webbook
rinpol	1871.00		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1871.00		NIST Webbook
tb	600.91	K	Joback Method
tc	809.91	K	Joback Method
tf	379.84	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.22	J/mol×K	600.91	Joback Method
cpg	605.30	J/mol×K	635.74	Joback Method
cpg	626.99	J/mol×K	670.58	Joback Method
cpg	647.37	J/mol×K	705.41	Joback Method
cpg	666.55	J/mol×K	740.24	Joback Method
cpg	684.60	J/mol×K	775.07	Joback Method
cpg	701.64	J/mol×K	809.91	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R208012&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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