4,8-diethyl-2-thiaadamantane

Inchi: InChI=1S/C13H22S/c1-3-10-8-5-9-7-12(10)14-13(6-8)11(9)4-2/h8-13H,3-7H2,1-2H3
InchiKey: HMDMYPGLMLNKOS-UHFFFAOYSA-N
Formula: C13H22S
SMILES: CCC1C2CC3CC1SC(C2)C3CC
Mol. weight [g/mol]: 210.38

Physical Properties

Property code	Value	Unit	Source
gf	245.46	kJ/mol	Joback Method
hf	-115.17	kJ/mol	Joback Method
hfus	28.60	kJ/mol	Joback Method
hvap	49.33	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.953		Crippen Method
mcvol	177.800	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	1746.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1718.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1718.00		NIST Webbook
tb	555.15	K	Joback Method
tc	771.22	K	Joback Method
tf	357.30	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.44	J/mol×K	555.15	Joback Method
cpg	498.11	J/mol×K	591.16	Joback Method
cpg	519.33	J/mol×K	627.17	Joback Method
cpg	539.22	J/mol×K	663.18	Joback Method
cpg	557.85	J/mol×K	699.19	Joback Method
cpg	575.33	J/mol×K	735.21	Joback Method
cpg	591.74	J/mol×K	771.22	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R207980&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
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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