4,8-dimethyl-2-thiaadamantane

Inchi: InChI=1S/C11H18S/c1-6-8-3-9-5-10(6)12-11(4-8)7(9)2/h6-11H,3-5H2,1-2H3
InchiKey: LOTVPGBDKCHZJQ-UHFFFAOYSA-N
Formula: C11H18S
SMILES: CC1C2CC3CC1SC(C2)C3C
Mol. weight [g/mol]: 182.33

Physical Properties

Property code	Value	Unit	Source
gf	228.62	kJ/mol	Joback Method
hf	-73.89	kJ/mol	Joback Method
hfus	23.42	kJ/mol	Joback Method
hvap	44.88	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.172		Crippen Method
mcvol	149.620	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1559.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1559.00		NIST Webbook
tb	509.39	K	Joback Method
tc	733.08	K	Joback Method
tf	334.76	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.53	J/mol×K	509.39	Joback Method
cpg	396.46	J/mol×K	546.67	Joback Method
cpg	416.92	J/mol×K	583.95	Joback Method
cpg	436.00	J/mol×K	621.23	Joback Method
cpg	453.80	J/mol×K	658.51	Joback Method
cpg	470.42	J/mol×K	695.80	Joback Method
cpg	485.95	J/mol×K	733.08	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R208007&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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