4,8-diethylidene-2-thiaadamantane

Inchi: InChI=1S/C13H18S/c1-3-10-8-5-9-7-12(10)14-13(6-8)11(9)4-2/h3-4,8-9,12-13H,5-7H2,1-
InchiKey: DQYPQUPLZVFUDV-HULALXFYSA-N
Formula: C13H18S
SMILES: CC=C1C2CC3CC1SC(C2)C3=CC
Mol. weight [g/mol]: 206.35

Physical Properties

Property code	Value	Unit	Source
gf	351.80	kJ/mol	Joback Method
hf	77.57	kJ/mol	Joback Method
hfus	27.11	kJ/mol	Joback Method
hvap	51.52	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.793		Crippen Method
mcvol	169.200	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1679.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1679.00		NIST Webbook
tb	577.77	K	Joback Method
tc	808.16	K	Joback Method
tf	386.50	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.51	J/mol×K	577.77	Joback Method
cpg	455.93	J/mol×K	616.17	Joback Method
cpg	473.97	J/mol×K	654.57	Joback Method
cpg	490.76	J/mol×K	692.97	Joback Method
cpg	506.43	J/mol×K	731.37	Joback Method
cpg	521.12	J/mol×K	769.76	Joback Method
cpg	534.96	J/mol×K	808.16	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R207995&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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