1,3-Dibromo-5,7-dimethyladamantane

Other names: 5,7-dimethyl-1,3-dibromoadamantane
Inchi: InChI=1S/C12H18Br2/c1-9-3-10(2)6-11(13,4-9)8-12(14,5-9)7-10/h3-8H2,1-2H3
InchiKey: XIWKEBIXYLMOKD-UHFFFAOYSA-N
Formula: C12H18Br2
SMILES: CC12CC3(C)CC(Br)(C1)CC(Br)(C2)C3
Mol. weight [g/mol]: 322.08

Physical Properties

Property code	Value	Unit	Source
gf	219.28	kJ/mol	Joback Method
hf	14.51	kJ/mol	Joback Method
hfus	5.59	kJ/mol	Joback Method
hvap	50.17	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.648		Crippen Method
mcvol	182.360	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
rinpol	1642.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	627.06	K	Joback Method
tc	903.97	K	Joback Method
tf	486.26	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.45	J/mol×K	627.06	Joback Method
cpg	475.71	J/mol×K	673.21	Joback Method
cpg	492.27	J/mol×K	719.36	Joback Method
cpg	509.08	J/mol×K	765.51	Joback Method
cpg	527.11	J/mol×K	811.66	Joback Method

cpg	547.32	J/mol×K	857.82	Joback Method
cpg	570.67	J/mol×K	903.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U411416&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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