

1,3,5-Tribromoadamantane

Inchi:	InChI=1S/C10H13Br3/c11-8-1-7-2-9(12,4-8)6-10(13,3-7)5-8/h7H,1-6H2
InchiKey:	WZCLLQRZXWUEOP-UHFFFAOYSA-N
Formula:	C10H13Br3
SMILES:	BrC12CC3CC(Br)(C1)CC(Br)(C3)C2
Mol. weight [g/mol]:	372.92

Physical Properties

Property code	Value	Unit	Source
gf	222.25	kJ/mol	Joback Method
hf	66.88	kJ/mol	Joback Method
hfus	11.99	kJ/mol	Joback Method
hvap	53.31	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.385		Crippen Method
mcvol	171.680	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
rinpol	1779.00		NIST Webbook
rinpol	1779.00		NIST Webbook
rinpol	1779.00		NIST Webbook
ripol	2659.00		NIST Webbook
ripol	2659.00		NIST Webbook
ripol	2659.00		NIST Webbook
tb	647.22	K	Joback Method
tc	939.65	K	Joback Method
tf	499.62	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.71	J/molxK	647.22	Joback Method
cpg	414.18	J/molxK	695.96	Joback Method
cpg	428.24	J/molxK	744.70	Joback Method
cpg	442.83	J/molxK	793.44	Joback Method

cpg	458.88	J/mol×K	842.18	Joback Method
cpg	477.33	J/mol×K	890.92	Joback Method
cpg	499.11	J/mol×K	939.65	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U411478&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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