1,3-Difluoroadamantane

Inchi: InChI=1S/C10H14F2/c11-9-2-7-1-8(4-9)5-10(12,3-7)6-9/h7-8H,1-6H2/t7-,8+,9+,10-
InchiKey: BWHJRYOYZZDMLO-FIRGSJFUSA-N
Formula: C10H14F2
SMILES: FC12CC3CC(C1)CC(F)(C3)C2
Mol. weight [g/mol]: 172.22

Physical Properties

Property code	Value	Unit	Source
gf	-204.84	kJ/mol	Joback Method
hf	-419.57	kJ/mol	Joback Method
hfus	8.60	kJ/mol	Joback Method
hvap	33.52	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.017		Crippen Method
mcvol	122.720	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1135.00		NIST Webbook
rinpol	1135.00		NIST Webbook
tb	447.04	K	Joback Method
tc	655.72	K	Joback Method
tf	297.50	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.48	J/mol×K	447.04	Joback Method
cpg	310.44	J/mol×K	481.82	Joback Method
cpg	328.47	J/mol×K	516.60	Joback Method
cpg	344.81	J/mol×K	551.38	Joback Method
cpg	359.71	J/mol×K	586.16	Joback Method
cpg	373.40	J/mol×K	620.94	Joback Method
cpg	386.13	J/mol×K	655.72	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=R405208&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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