1-Fluoroadamantane

Inchi: InChI=1S/C10H15F/c11-10-4-7-1-8(5-10)3-9(2-7)6-10/h7-9H,1-6H2
InchiKey: CPWSNJSGSXXVLD-UHFFFAOYSA-N
Formula: C10H15F
SMILES: FC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 154.22
CAS: 768-92-3

Physical Properties

Property code	Value	Unit	Source
gf	-4.54	kJ/mol	Joback Method
hf	-238.70	kJ/mol	Joback Method
hfus	11.81	kJ/mol	Joback Method
hvap	35.49	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.925		Crippen Method
mcvol	120.950	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1159.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1159.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1534.00		NIST Webbook
ripol	1512.00		NIST Webbook
ripol	1512.00		NIST Webbook
tb	447.53	K	Joback Method
tc	658.65	K	Joback Method
tf	525.00 ± 1.00	K	NIST Webbook
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.51	J/mol×K	447.53	Joback Method
cpg	302.00	J/mol×K	482.72	Joback Method
cpg	320.80	J/mol×K	517.90	Joback Method
cpg	338.08	J/mol×K	553.09	Joback Method
cpg	354.00	J/mol×K	588.28	Joback Method
cpg	368.73	J/mol×K	623.47	Joback Method
cpg	382.45	J/mol×K	658.65	Joback Method
hfust	1.50	kJ/mol	221.60	NIST Webbook

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=C768923&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
hfust:	Enthalpy of fusion at a given temperature
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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