2-fluoroadamantane

Inchi: InChI=1S/C10H15F/c11-10-8-2-6-1-7(4-8)5-9(10)3-6/h6-10H,1-5H2
InchiKey: SVIIPBADUQGZCF-UHFFFAOYSA-N
Formula: C10H15F
SMILES: FC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 154.22
CAS: 16668-83-0

Physical Properties

Property code	Value	Unit	Source
gf	-6.76	kJ/mol	Joback Method
hf	-274.28	kJ/mol	Joback Method
hfus	19.18	kJ/mol	Joback Method
hvap	36.33	kJ/mol	Joback Method
ie	9.46	eV	NIST Webbook
log10ws	-2.69		Crippen Method
logp	2.781		Crippen Method
mcvol	120.950	ml/mol	McGowan Method
pc	2847.48	kPa	Joback Method
rinpol	1210.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1544.00		NIST Webbook
ripol	1521.00		NIST Webbook
tb	442.62	K	Joback Method
tc	644.36	K	Joback Method
tf	244.87	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.41	J/mol×K	442.62	Joback Method
cpg	300.79	J/mol×K	476.24	Joback Method
cpg	319.86	J/mol×K	509.87	Joback Method
cpg	337.71	J/mol×K	543.49	Joback Method
cpg	354.40	J/mol×K	577.11	Joback Method
cpg	370.01	J/mol×K	610.73	Joback Method
cpg	384.62	J/mol×K	644.36	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16668830&Units=SI

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
ie: Ionization energy
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