Buturon, HFBA

Inchi: InChI=1S/C16H12ClF7N2O2/c1-4-9(2)25(3)13(28)26(11-7-5-10(17)6-8-11)12(27)14(18,1
InchiKey: FNMKVFLBRBGPFD-UHFFFAOYSA-N
Formula: C16H12ClF7N2O2
SMILES: C#CC(C)N(C)C(=O)N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccc(Cl)cc1
Mol. weight [g/mol]: 432.72

Physical Properties

Property code	Value	Unit	Source
gf	-996.11	kJ/mol	Joback Method
hf	-1366.75	kJ/mol	Joback Method
hfus	43.05	kJ/mol	Joback Method
hvap	65.97	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.579		Crippen Method
mcvol	251.670	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	1653.00		NIST Webbook
rinpol	1653.00		NIST Webbook
tb	742.07	K	Joback Method
tc	935.56	K	Joback Method
tf	547.10	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.94	J/mol×K	742.07	Joback Method
cpg	723.24	J/mol×K	774.32	Joback Method
cpg	733.63	J/mol×K	806.57	Joback Method
cpg	743.19	J/mol×K	838.82	Joback Method
cpg	752.03	J/mol×K	871.06	Joback Method
cpg	760.27	J/mol×K	903.31	Joback Method
cpg	768.00	J/mol×K	935.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R220225&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