Fenuron, HFBA

Inchi: InChI=1S/C13H11F7N2O2/c1-21(2)10(24)22(8-6-4-3-5-7-8)9(23)11(14,15)12(16,17)13(1
InchiKey: PXPKBXKIKFRCLC-UHFFFAOYSA-N
Formula: C13H11F7N2O2
SMILES: CN(C)C(=O)N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccccc1
Mol. weight [g/mol]: 360.23

Physical Properties

Property code	Value	Unit	Source
gf	-1220.44	kJ/mol	Joback Method
hf	-1564.24	kJ/mol	Joback Method
hfus	32.02	kJ/mol	Joback Method
hvap	54.78	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.534		Crippen Method
mcvol	205.760	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	1501.00		NIST Webbook
tb	641.34	K	Joback Method
tc	822.05	K	Joback Method
tf	438.88	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.06	J/mol×K	641.34	Joback Method
cpg	590.74	J/mol×K	671.46	Joback Method
cpg	602.40	J/mol×K	701.58	Joback Method
cpg	613.12	J/mol×K	731.69	Joback Method
cpg	622.96	J/mol×K	761.81	Joback Method
cpg	632.02	J/mol×K	791.93	Joback Method
cpg	640.37	J/mol×K	822.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R220334&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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