Fenoxanil, N-heptafluorobutyryl-

Inchi: InChI=1S/C19H17Cl2F7N2O3/c1-9(2)16(4,8-29)30(15(32)17(22,23)18(24,25)19(26,27)2
InchiKey: RVRKBSHEASGOGO-UHFFFAOYSA-N
Formula: C19H17Cl2F7N2O3
SMILES: CC(Oc1ccc(Cl)cc1Cl)C(=O)N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)(C#N)C(C)C
Mol. weight [g/mol]: 525.25

Physical Properties

Property code	Value	Unit	Source
gf	-1297.68	kJ/mol	Joback Method
hf	-1796.68	kJ/mol	Joback Method
hfus	40.39	kJ/mol	Joback Method
hvap	87.00	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	5.887		Crippen Method
mcvol	312.050	ml/mol	McGowan Method
pc	1144.44	kPa	Joback Method
rinpol	2069.00		NIST Webbook
rinpol	2069.00		NIST Webbook
tb	971.39	K	Joback Method
tc	1191.71	K	Joback Method
tf	618.55	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.33	J/mol×K	971.39	Joback Method
cpg	961.08	J/mol×K	1008.11	Joback Method
cpg	970.30	J/mol×K	1044.83	Joback Method
cpg	979.12	J/mol×K	1081.55	Joback Method
cpg	987.69	J/mol×K	1118.27	Joback Method
cpg	996.17	J/mol×K	1154.99	Joback Method
cpg	1004.70	J/mol×K	1191.71	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=U374339&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
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