N-(2-Pentafluoropropionyloxy-1-phenyl-ethyl)-ber

Inchi: InChI=1S/C17H14F5NO4S/c18-16(19,17(20,21)22)15(24)27-11-14(12-7-3-1-4-8-12)23-2
InchiKey: RBHCTTUDMRKDFZ-UHFFFAOYSA-N
Formula: C17H14F5NO4S
SMILES: O=C(OCC(NS(=O)(=O)c1ccccc1)c1ccccc1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 423.35

Physical Properties

Property code	Value	Unit	Source
gf	-1266.80	kJ/mol	Joback Method
hf	-1569.16	kJ/mol	Joback Method
hfus	44.18	kJ/mol	Joback Method
hvap	85.15	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.447		Crippen Method
mcvol	257.230	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
tb	805.41	K	Joback Method
tc	1011.33	K	Joback Method
tf	490.36	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.09	J/mol×K	805.41	Joback Method
cpg	770.09	J/mol×K	839.73	Joback Method
cpg	780.92	J/mol×K	874.05	Joback Method
cpg	790.65	J/mol×K	908.37	Joback Method
cpg	799.36	J/mol×K	942.69	Joback Method
cpg	807.10	J/mol×K	977.01	Joback Method
cpg	813.96	J/mol×K	1011.33	Joback Method

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=U374417&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
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