N-(2-Heptafluorobutyryloxy-1-phenyl-ethyl)-benze

Inchi: InChI=1S/C18H14F7NO4S/c19-16(20,17(21,22)18(23,24)25)15(27)30-11-14(12-7-3-1-4-
InchiKey: UTKQSXIQWFVXOY-UHFFFAOYSA-N
Formula: C18H14F7NO4S
SMILES: O=C(OCC(NS(=O)(=O)c1ccccc1)c1ccccc1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 473.36

Physical Properties

Property code	Value	Unit	Source
gf	-1645.16	kJ/mol	Joback Method
hf	-1990.77	kJ/mol	Joback Method
hfus	45.52	kJ/mol	Joback Method
hvap	84.45	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.082		Crippen Method
mcvol	274.860	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	2240.00		NIST Webbook
tb	823.60	K	Joback Method
tc	1024.62	K	Joback Method
tf	505.23	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.08	J/mol×K	823.60	Joback Method
cpg	841.54	J/mol×K	857.10	Joback Method
cpg	851.89	J/mol×K	890.61	Joback Method
cpg	861.21	J/mol×K	924.11	Joback Method
cpg	869.59	J/mol×K	957.61	Joback Method
cpg	877.13	J/mol×K	991.12	Joback Method
cpg	883.90	J/mol×K	1024.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374418&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