Nitrobenzene, 3-heptafluorobutyrylamino-4-heptafluorobutyrylox

Inchi: InChI=1S/C14H4F14N2O5/c15-9(16,11(19,20)13(23,24)25)7(31)29-5-3-4(30(33)34)1-2-6

InchiKey: NUZGOEGSDOPLEA-UHFFFAOYSA-N

Formula: C14H4F14N2O5

SMILES: O=C(Nc1cc([N+](=O)[O-])ccc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 546.17

Physical Properties

Property code	Value	Unit	Source
gf	-2788.05	kJ/mol	Joback Method
hf	-3231.41	kJ/mol	Joback Method
hfus	44.76	kJ/mol	Joback Method
hvap	70.07	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	5.104		Crippen Method
mcvol	245.550	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
tb	858.93	K	Joback Method
tc	1055.26	K	Joback Method
tf	640.14	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.72	J/mol×K	858.93	Joback Method
cpg	785.49	J/mol×K	891.65	Joback Method
cpg	791.69	J/mol×K	924.37	Joback Method
cpg	797.42	J/mol×K	957.09	Joback Method
cpg	802.82	J/mol×K	989.81	Joback Method
cpg	808.01	J/mol×K	1022.53	Joback Method
cpg	813.12	J/mol×K	1055.26	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=U374263&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