2-((2,2,3,3,4,4,4-Heptafluorobutanoyl)amino)phenyl 2,2,3,3,4,4,4-heptafluorobutanoate

Inchi: InChI=1S/C14H5F14NO3/c15-9(16,11(19,20)13(23,24)25)7(30)29-5-3-1-2-4-6(5)32-8(31)10(17,18)12(21,22)14(26,27)28/h1-4H,(H,29,30)

InchiKey: RDWBQWPWKZRRHL-UHFFFAOYSA-N

Formula: C14H5F14NO3

SMILES: O=C(Nc1ccccc1OC(=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]: 501.17

Physical Properties

Property code	Value	Unit	Source
gf	-2813.97	kJ/mol	Joback Method
hf	-3209.18	kJ/mol	Joback Method
hfus	33.79	kJ/mol	Joback Method
hvap	52.82	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.196		Crippen Method
mcvol	228.130	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
rinpol	1231.00		NIST Webbook
rinpol	1231.00		NIST Webbook
tb	702.11	K	Joback Method
tc	870.94	K	Joback Method
tf	484.01	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.74	J/mol×K	702.11	Joback Method
cpg	703.11	J/mol×K	730.25	Joback Method
cpg	711.63	J/mol×K	758.39	Joback Method
cpg	719.37	J/mol×K	786.52	Joback Method
cpg	726.42	J/mol×K	814.66	Joback Method
cpg	732.86	J/mol×K	842.80	Joback Method
cpg	738.76	J/mol×K	870.94	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=U373276&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