

2,2,3,3,4,4,4-Heptafluoro-N-[4-(2,2,3,3,4,4,4-heptafluoro-N-oxo-1,2,3,4-tetrahydro-1H-benzothiazol-5-yl)phenyl]acetamide

Inchi: InChI=1S/C14H6F14N2O2/c15-9(16,11(19,20)13(23,24)25)7(31)29-5-1-2-6(4-3-5)30-8(3)
InchiKey: IHIMECRMQYQKJO-UHFFFAOYSA-N
Formula: C14H6F14N2O2
SMILES: O=C(Nc1ccc(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 500.19

Physical Properties

Property code	Value	Unit	Source
gf	-2619.58	kJ/mol	Joback Method
hf	-3023.49	kJ/mol	Joback Method
hfus	37.70	kJ/mol	Joback Method
hvap	56.85	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.229		Crippen Method
mcvol	232.240	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
rinpol	1632.00		NIST Webbook
rinpol	1632.00		NIST Webbook
tb	729.86	K	Joback Method
tc	902.60	K	Joback Method
tf	514.44	K	Joback Method
vc	0.980	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.39	J/molxK	729.86	Joback Method
cpg	727.41	J/molxK	758.65	Joback Method
cpg	735.60	J/molxK	787.44	Joback Method
cpg	743.05	J/molxK	816.23	Joback Method
cpg	749.87	J/molxK	845.02	Joback Method
cpg	756.14	J/molxK	873.81	Joback Method
cpg	761.97	J/molxK	902.60	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U373017&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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