L-Glutamine, N(«alpha»)-trifluoroacetyl-, 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C10H10F8N2O4/c11-8(12,10(16,17)18)3-24-6(22)4(1-2-5(19)21)20-7(23)9(13,

InchiKey: HHVFRVCGLBJKGR-UHFFFAOYSA-N

Formula: C10H10F8N2O4

SMILES: NC(=O)CCC(NC(=O)C(F)(F)F)C(=O)OCC(F)(F)C(F)(F)F

Mol. weight [g/mol]: 374.18

Physical Properties

Property code	Value	Unit	Source
gf	-1855.00	kJ/mol	Joback Method
hf	-2232.84	kJ/mol	Joback Method
hfus	36.81	kJ/mol	Joback Method
hvap	66.77	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	1.040		Crippen Method
mcvol	196.460	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	1552.70		NIST Webbook
rinpol	1552.70		NIST Webbook
tb	718.96	K	Joback Method
tc	894.93	K	Joback Method
tf	507.38	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.21	J/mol×K	718.96	Joback Method
cpg	600.36	J/mol×K	748.29	Joback Method
cpg	608.83	J/mol×K	777.62	Joback Method
cpg	616.64	J/mol×K	806.94	Joback Method
cpg	623.85	J/mol×K	836.27	Joback Method
cpg	630.50	J/mol×K	865.60	Joback Method
cpg	636.64	J/mol×K	894.93	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=U352338&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