L-Glutamic acid, N-trifluoroacetyl-, bis(2,2,3,3,3-pentafluoropropyl) ester

Inchi: InChI=1S/C13H10F13NO5/c14-9(15,12(21,22)23)3-31-6(28)2-1-5(27-8(30)11(18,19)20)7

InchiKey: RAALFVHWLBEPBO-UHFFFAOYSA-N

Formula: C13H10F13NO5

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

Mol. weight [g/mol]: 507.20

Physical Properties

Property code	Value	Unit	Source
gf	-2969.56	kJ/mol	Joback Method
hf	-3458.82	kJ/mol	Joback Method
hfus	41.14	kJ/mol	Joback Method
hvap	58.54	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.295		Crippen Method
mcvol	243.470	ml/mol	McGowan Method
pc	1293.93	kPa	Joback Method
rinpol	1255.20		NIST Webbook
rinpol	1255.20		NIST Webbook
tb	727.38	K	Joback Method
tc	891.90	K	Joback Method
tf	487.95	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.63	J/mol×K	727.38	Joback Method
cpg	768.67	J/mol×K	754.80	Joback Method
cpg	777.95	J/mol×K	782.22	Joback Method
cpg	786.50	J/mol×K	809.64	Joback Method
cpg	794.40	J/mol×K	837.06	Joback Method
cpg	801.69	J/mol×K	864.48	Joback Method
cpg	808.44	J/mol×K	891.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352354&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