allo-threonine, trifluoroacetyl-isopropyl ester

Inchi: InChI=1S/C11H13F6NO5/c1-4(2)22-7(19)6(18-8(20)10(12,13)14)5(3)23-9(21)11(15,16)1
InchiKey: BQCCNVGQXRSHIG-NTSWFWBYSA-N
Formula: C11H13F6NO5
SMILES: CC(C)OC(=O)C(NC(=O)C(F)(F)F)C(C)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 353.21

Physical Properties

Property code	Value	Unit	Source
gf	-1636.13	kJ/mol	Joback Method
hf	-2029.08	kJ/mol	Joback Method
hfus	29.60	kJ/mol	Joback Method
hvap	62.92	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	1.479		Crippen Method
mcvol	202.900	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
rinpol	1203.00		NIST Webbook
tb	695.54	K	Joback Method
tc	870.65	K	Joback Method
tf	424.02	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.62	J/mol×K	695.54	Joback Method
cpg	602.69	J/mol×K	724.72	Joback Method
cpg	613.04	J/mol×K	753.91	Joback Method
cpg	622.68	J/mol×K	783.09	Joback Method
cpg	631.64	J/mol×K	812.28	Joback Method
cpg	639.95	J/mol×K	841.46	Joback Method
cpg	647.63	J/mol×K	870.65	Joback Method

Sources

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=R267828&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:
https://www.chemeo.com/cid/32-434-4/allo-threonine-trifluoroacetyl-isopropyl-ester.pdf
Generated by Cheméo on 2024-04-20 08:40:15.831475283 +0000 UTC m=+15891664.752052596.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.