Glutamine, N-trifluoroacetyl, 1-methylethyl ester

Inchi: InChI=1S/C10H15F3N2O4/c1-5(2)19-8(17)6(3-4-7(14)16)15-9(18)10(11,12)13/h5-6H,3-4

InchiKey: IHJANNQLLFLEOG-UHFFFAOYSA-N

Formula: C10H15F3N2O4

SMILES: CC(C)OC(=O)C(CCC(N)=O)NC(=O)C(F)(F)F

Mol. weight [g/mol]: 284.23

Physical Properties

Property code	Value	Unit	Source
gf	-889.07	kJ/mol	Joback Method
hf	-1240.07	kJ/mol	Joback Method
hfus	32.72	kJ/mol	Joback Method
hvap	73.06	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	0.251		Crippen Method
mcvol	187.610	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1518.00		NIST Webbook
tb	728.63	K	Joback Method
tc	920.58	K	Joback Method
tf	484.59	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.73	J/mol×K	728.63	Joback Method
cpg	557.64	J/mol×K	760.62	Joback Method
cpg	567.80	J/mol×K	792.61	Joback Method
cpg	577.24	J/mol×K	824.60	Joback Method
cpg	585.99	J/mol×K	856.59	Joback Method
cpg	594.08	J/mol×K	888.59	Joback Method
cpg	601.52	J/mol×K	920.58	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=R84392&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