N-(Heptafluorobutyryl)methionine propyl ester

Other names: L-Methionine, N-heptafluorobutyryl-, propyl ester
Inchi: InChI=1S/C12H16F7NO3S/c1-3-5-23-8(21)7(4-6-24-2)20-9(22)10(13,14)11(15,16)12(17,
InchiKey: DXEDYBBAJBCCRO-UHFFFAOYSA-N
Formula: C12H16F7NO3S
SMILES: CCCOC(=O)C(CCSC)NC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 387.31
CAS: 88436-11-7

Physical Properties

Property code	Value	Unit	Source
gf	-1547.76	kJ/mol	Joback Method
hf	-1957.35	kJ/mol	Joback Method
hfus	36.25	kJ/mol	Joback Method
hvap	61.47	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.010		Crippen Method
mcvol	227.670	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	1550.00		NIST Webbook
tb	707.83	K	Joback Method
tc	884.98	K	Joback Method
tf	430.54	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.77	J/mol×K	707.83	Joback Method
cpg	677.66	J/mol×K	737.35	Joback Method
cpg	688.74	J/mol×K	766.88	Joback Method
cpg	699.05	J/mol×K	796.40	Joback Method
cpg	708.63	J/mol×K	825.93	Joback Method
cpg	717.54	J/mol×K	855.45	Joback Method
cpg	725.81	J/mol×K	884.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88436117&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