l-Methionine, n-heptafluorobutyryl-, hexyl ester

Inchi: InChI=1S/C15H22F7NO3S/c1-3-4-5-6-8-26-11(24)10(7-9-27-2)23-12(25)13(16,17)14(18

InchiKey: SYZFLABRJFVDFZ-UHFFFAOYSA-N

Formula: C15H22F7NO3S

SMILES: CCCCCCOC(=O)C(CCSC)NC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 429.39

Physical Properties

Property code	Value	Unit	Source
gf	-1522.50	kJ/mol	Joback Method
hf	-2019.27	kJ/mol	Joback Method
hfus	44.02	kJ/mol	Joback Method
hvap	68.14	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.181		Crippen Method
mcvol	269.940	ml/mol	McGowan Method
pc	1304.23	kPa	Joback Method
rinpol	1801.00		NIST Webbook
rinpol	1801.00		NIST Webbook
tb	776.47	K	Joback Method
tc	956.96	K	Joback Method
tf	464.35	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.06	J/mol×K	776.47	Joback Method
cpg	842.13	J/mol×K	806.55	Joback Method
cpg	854.33	J/mol×K	836.63	Joback Method
cpg	865.70	J/mol×K	866.72	Joback Method
cpg	876.32	J/mol×K	896.80	Joback Method
cpg	886.22	J/mol×K	926.88	Joback Method
cpg	895.46	J/mol×K	956.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320855&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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