l-Methionine, n-heptafluorobutyryl-, isohexyl ester

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

InchiKey: PPYXFSQWZOAGNC-UHFFFAOYSA-N

Formula: C15H22F7NO3S

SMILES: CSCCC(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(=O)OCCCC(C)C

Mol. weight [g/mol]: 429.39

Physical Properties

Property code	Value	Unit	Source
gf	-1524.94	kJ/mol	Joback Method
hf	-2024.55	kJ/mol	Joback Method
hfus	40.49	kJ/mol	Joback Method
hvap	67.76	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.037		Crippen Method
mcvol	269.940	ml/mol	McGowan Method
pc	1311.80	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	776.03	K	Joback Method
tc	957.75	K	Joback Method
tf	449.35	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.61	J/mol×K	776.03	Joback Method
cpg	842.78	J/mol×K	806.32	Joback Method
cpg	855.05	J/mol×K	836.60	Joback Method
cpg	866.49	J/mol×K	866.89	Joback Method
cpg	877.14	J/mol×K	897.18	Joback Method
cpg	887.06	J/mol×K	927.47	Joback Method
cpg	896.31	J/mol×K	957.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320854&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