l-Leucine, N-neopentyloxycarbonyl-N-methyl-, neopentyl ester

Inchi: InChI=1S/C18H35NO4/c1-13(2)10-14(15(20)22-11-17(3,4)5)19(9)16(21)23-12-18(6,7)8/h
InchiKey: OCUYRQWPXLJKBP-UHFFFAOYSA-N
Formula: C18H35NO4
SMILES: CC(C)CC(C(=O)OCC(C)(C)C)N(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]: 329.47

Physical Properties

Property code	Value	Unit	Source
gf	-255.58	kJ/mol	Joback Method
hf	-864.98	kJ/mol	Joback Method
hfus	29.10	kJ/mol	Joback Method
hvap	72.65	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	4.105		Crippen Method
mcvol	289.340	ml/mol	McGowan Method
pc	1273.69	kPa	Joback Method
tb	768.92	K	Joback Method
tc	960.09	K	Joback Method
tf	444.25	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.86	J/mol×K	768.92	Joback Method
cpg	914.10	J/mol×K	800.78	Joback Method
cpg	931.24	J/mol×K	832.64	Joback Method
cpg	947.32	J/mol×K	864.51	Joback Method
cpg	962.39	J/mol×K	896.37	Joback Method
cpg	976.50	J/mol×K	928.23	Joback Method
cpg	989.71	J/mol×K	960.09	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321920&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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