L-Valine, N-(2-methoxybenzoyl)-, propyl ester

Inchi: InChI=1S/C16H23NO4/c1-5-10-21-16(19)14(11(2)3)17-15(18)12-8-6-7-9-13(12)20-4/h6-9
InchiKey: DDHZEEMBYBDWJU-UHFFFAOYSA-N
Formula: C16H23NO4
SMILES: CCCOC(=O)C(NC(=O)c1ccccc1OC)C(C)C
Mol. weight [g/mol]: 293.36

Physical Properties

Property code	Value	Unit	Source
gf	-196.71	kJ/mol	Joback Method
hf	-595.20	kJ/mol	Joback Method
hfus	34.48	kJ/mol	Joback Method
hvap	78.12	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.403		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
rinpol	2208.00		NIST Webbook
rinpol	2208.00		NIST Webbook
tb	799.01	K	Joback Method
tc	1007.86	K	Joback Method
tf	476.00	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.79	J/mol×K	799.01	Joback Method
cpg	720.56	J/mol×K	833.82	Joback Method
cpg	734.23	J/mol×K	868.63	Joback Method
cpg	746.82	J/mol×K	903.43	Joback Method
cpg	758.34	J/mol×K	938.24	Joback Method
cpg	768.82	J/mol×K	973.05	Joback Method
cpg	778.26	J/mol×K	1007.86	Joback Method

Sources

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=U346589&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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