DL-tert-leucine

Inchi: InChI=1S/C6H13NO2/c1-6(2,3)4(7)5(8)9/h4H,7H2,1-3H3,(H,8,9)
InchiKey: NPDBDJFLKKQMCM-UHFFFAOYSA-N
Formula: C6H13NO2
SMILES: CC(C)(C)C(N)C(=O)O
Mol. weight [g/mol]: 131.17

Physical Properties

Property code	Value	Unit	Source
hf	-515.91	kJ/mol	Cheméo Relay (1.0)
hfus	11.24	kJ/mol	Joback Method
ie	8.62	eV	Cheméo Relay (1.0)
log10ws	-0.60		Cheméo Relay (1.0)
logp	0.444		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
tf	507.37	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.04	J/mol×K	551.59	Joback Method
cpg	289.06	J/mol×K	584.22	Joback Method
cpg	298.49	J/mol×K	616.86	Joback Method
cpg	307.34	J/mol×K	649.49	Joback Method
cpg	315.66	J/mol×K	682.13	Joback Method
cpg	323.46	J/mol×K	714.76	Joback Method
cpg	330.79	J/mol×K	747.40	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Infinite Dilution Binary Diffusion Coefficients of Several r-Amino Acids in Water over a Temperature Range from (293.2 to 333.2) K with the Taylor Dispersion Technique:	https://www.doi.org/10.1021/je060149b

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point