(Dl)-2-amino-2-methyl-butanoic acid

Inchi: InChI=1S/C5H11NO2/c1-3-5(2,6)4(7)8/h3,6H2,1-2H3,(H,7,8)
InchiKey: GCHPUFAZSONQIV-UHFFFAOYSA-N
Formula: C5H11NO2
SMILES: CCC(C)(N)C(=O)O
Mol. weight [g/mol]: 117.15
CAS: 465-58-7

Physical Properties

Property code	Value	Unit	Source
gf	-205.23	kJ/mol	Joback Method
hf	-386.30	kJ/mol	Joback Method
hfus	12.18	kJ/mol	Joback Method
hvap	59.49	kJ/mol	Joback Method
log10ws	-0.56		Crippen Method
logp	0.198		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
tb	529.15	K	Joback Method
tc	723.51	K	Joback Method
tf	342.54	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.41	J/mol×K	529.15	Joback Method
cpg	244.22	J/mol×K	561.54	Joback Method
cpg	252.51	J/mol×K	593.94	Joback Method
cpg	260.29	J/mol×K	626.33	Joback Method
cpg	267.59	J/mol×K	658.72	Joback Method
cpg	274.45	J/mol×K	691.12	Joback Method
cpg	280.88	J/mol×K	723.51	Joback Method
hsubt	134.00 ± 1.00	kJ/mol	413.00	NIST Webbook
hsubt	125.80 ± 0.40	kJ/mol	454.00	NIST Webbook

Sources

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=C465587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hsubt:	Enthalpy of sublimation at a given temperature
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