

Aspartic acid, dimethyl ester

Other names:	dimethyl DL-aspartate
Inchi:	InChI=1S/C6H11NO4/c1-10-5(8)3-4(7)6(9)11-2/h4H,3,7H2,1-2H3
InchiKey:	BYHXBBOSJKPUJL-UHFFFAOYSA-N
Formula:	C6H11NO4
SMILES:	COC(=O)CC(N)C(=O)OC
Mol. weight [g/mol]:	161.16
CAS:	40149-67-5

Physical Properties

Property code	Value	Unit	Source
gf	-404.19	kJ/mol	Joback Method
hf	-628.26	kJ/mol	Joback Method
hfus	18.54	kJ/mol	Joback Method
hvap	57.52	kJ/mol	Joback Method
log10ws	0.39		Crippen Method
logp	-0.950		Crippen Method
mcvol	120.260	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
tb	561.35	K	Joback Method
tc	763.20	K	Joback Method
tf	369.96	K	Joback Method
vc	0.443	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.38	J/mol×K	561.35	Joback Method
cpg	297.41	J/mol×K	594.99	Joback Method
cpg	307.01	J/mol×K	628.63	Joback Method
cpg	316.17	J/mol×K	662.27	Joback Method
cpg	324.86	J/mol×K	695.91	Joback Method
cpg	333.08	J/mol×K	729.56	Joback Method
cpg	340.82	J/mol×K	763.20	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=C40149675&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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