

n-Octylmalonic acid

Inchi:	InChI=1S/C11H20O4/c1-2-3-4-5-6-7-8-9(10(12)13)11(14)15/h9H,2-8H2,1H3,(H,12,13)(H
InchiKey:	QJGNSTCICFBACB-UHFFFAOYSA-N
Formula:	C11H20O4
SMILES:	CCCCCCCCC(C(=O)O)C(=O)O
Mol. weight [g/mol]:	216.27
CAS:	760-55-4

Physical Properties

Property code	Value	Unit	Source
chs	-6080.10 ± 2.90	kJ/mol	NIST Webbook
gf	-492.18	kJ/mol	Joback Method
hf	-805.27	kJ/mol	Joback Method
hfus	32.10	kJ/mol	Joback Method
hvap	86.54	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.522		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
tb	742.74	K	Joback Method
tc	919.59	K	Joback Method
tf	420.23	K	Joback Method
vc	0.696	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.61	J/mol×K	742.74	Joback Method
cpg	574.81	J/mol×K	890.12	Joback Method
cpg	566.22	J/mol×K	860.64	Joback Method
cpg	557.11	J/mol×K	831.17	Joback Method
cpg	547.49	J/mol×K	801.69	Joback Method
cpg	537.33	J/mol×K	772.22	Joback Method
cpg	582.93	J/mol×K	919.59	Joback Method
dvisc	0.0000111	Paxs	742.74	Joback Method

dvisc	0.0000194	Paxs	688.99	Joback Method
dvisc	0.0000373	Paxs	635.24	Joback Method
dvisc	0.0000808	Paxs	581.49	Joback Method
dvisc	0.0002051	Paxs	527.73	Joback Method
dvisc	0.0006428	Paxs	473.98	Joback Method
dvisc	0.0026981	Paxs	420.23	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=C760554&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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