

Gorlic acid

Inchi:	InChI=1S/C18H30O2/c19-18(20)16-10-8-6-4-2-1-3-5-7-9-13-17-14-11-12-15-17/h2,4,11,
InchiKey:	XADKGDBMULSEAC-DUXPYHPUSA-N
Formula:	C18H30O2
SMILES:	O=C(O)CCCCC=CCCCCCC1C=CCC1
Mol. weight [g/mol]:	278.43
CAS:	502-31-8

Physical Properties

Property code	Value	Unit	Source
gf	-18.33	kJ/mol	Joback Method
hf	-444.18	kJ/mol	Joback Method
hfus	43.42	kJ/mol	Joback Method
hvap	79.59	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.494		Crippen Method
mcvol	252.460	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2205.10		NIST Webbook
rinpol	2205.10		NIST Webbook
tb	775.89	K	Joback Method
tc	963.41	K	Joback Method
tf	409.95	K	Joback Method
vc	0.976	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.96	J/mol×K	775.89	Joback Method
cpg	793.35	J/mol×K	807.14	Joback Method
cpg	808.87	J/mol×K	838.40	Joback Method
cpg	823.55	J/mol×K	869.65	Joback Method
cpg	837.47	J/mol×K	900.90	Joback Method
cpg	850.66	J/mol×K	932.16	Joback Method
cpg	863.18	J/mol×K	963.41	Joback Method

dvisc	0.0024178	Paxs	409.95	Joback Method
dvisc	0.0007366	Paxs	470.94	Joback Method
dvisc	0.0002947	Paxs	531.93	Joback Method
dvisc	0.0001424	Paxs	592.92	Joback Method
dvisc	0.0000788	Paxs	653.91	Joback Method
dvisc	0.0000482	Paxs	714.90	Joback Method
dvisc	0.0000319	Paxs	775.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C502318&Units=SI

Legend

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
mvol:	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

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