1-«alpha»,2-«alpha»,5-«alpha»-Nepetonic acid, methyl ester

Inchi: InChI=1S/C11H18O3/c1-7-4-5-9(8(2)6-12)10(7)11(13)14-3/h6-10H,4-5H2,1-3H3/t7-,8?,9

InchiKey: PWAGNDORTYARTI-HFXXUHSDSA-N

Formula: C11H18O3

SMILES: COC(=O)C1C(C)CCC1C(C)C=O

Mol. weight [g/mol]: 198.26

Physical Properties

Property code	Value	Unit	Source
gf	-273.01	kJ/mol	Joback Method
hf	-586.23	kJ/mol	Joback Method
hfus	21.88	kJ/mol	Joback Method
hvap	55.21	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.657		Crippen Method
mcvol	164.000	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1303.00		NIST Webbook
rinpol	1303.00		NIST Webbook
tb	581.53	K	Joback Method
tc	784.31	K	Joback Method
tf	315.31	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.50	J/mol×K	581.53	Joback Method
cpg	447.67	J/mol×K	615.33	Joback Method
cpg	463.95	J/mol×K	649.12	Joback Method
cpg	479.34	J/mol×K	682.92	Joback Method
cpg	493.86	J/mol×K	716.72	Joback Method
cpg	507.51	J/mol×K	750.51	Joback Method
cpg	520.31	J/mol×K	784.31	Joback Method
dvisc	0.0028519	Pa×s	315.31	Joback Method

dvisc	0.0016749	Pa×s	359.68	Joback Method
dvisc	0.0011056	Pa×s	404.05	Joback Method
dvisc	0.0007923	Pa×s	448.42	Joback Method
dvisc	0.0006029	Pa×s	492.79	Joback Method
dvisc	0.0004800	Pa×s	537.16	Joback Method
dvisc	0.0003957	Pa×s	581.53	Joback Method

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=R197110&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume