Neocarvomenthyl acetate

Inchi: InChI=1S/C12H22O2/c1-8(2)11-6-5-9(3)12(7-11)14-10(4)13/h8-9,11-12H,5-7H2,1-4H3/t9
InchiKey: JAKFDYGDDRCJLY-DLOVCJGASA-N
Formula: C12H22O2
SMILES: CC(=O)OC1CC(C(C)C)CCC1C
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-177.17	kJ/mol	Joback Method
hf	-527.45	kJ/mol	Joback Method
hfus	20.08	kJ/mol	Joback Method
hvap	50.89	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	3.010		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1259.00		NIST Webbook
rinpol	1259.00		NIST Webbook
ripol	1604.00		NIST Webbook
ripol	1604.00		NIST Webbook
tb	560.02	K	Joback Method
tc	763.29	K	Joback Method
tf	281.06	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.30	J/mol×K	560.02	Joback Method
cpg	548.42	J/mol×K	729.41	Joback Method
cpg	531.98	J/mol×K	695.54	Joback Method
cpg	514.55	J/mol×K	661.66	Joback Method
cpg	496.13	J/mol×K	627.78	Joback Method
cpg	476.71	J/mol×K	593.90	Joback Method

cpg	563.88	J/mol×K	763.29	Joback Method
dvisc	0.0002379	Pa×s	560.02	Joback Method
dvisc	0.0003020	Pa×s	513.53	Joback Method
dvisc	0.0004019	Pa×s	467.03	Joback Method
dvisc	0.0005700	Pa×s	420.54	Joback Method
dvisc	0.0008815	Pa×s	374.05	Joback Method
dvisc	0.0015430	Pa×s	327.55	Joback Method
dvisc	0.0032505	Pa×s	281.06	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=R134075&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume