

Neoisomenthyl acetate

Inchi: InChI=1S/C12H22O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h8-9,11-12H,5-7H2,1-4H3/t9
InchiKey: XHXUANMFYXWVNG-YUSALJHKSA-N
Formula: C12H22O2
SMILES: CC(=O)OC1CC(C)CCC1C(C)C
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
ripol	1276.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1276.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1612.00		NIST Webbook
ripol	1612.00		NIST Webbook
ripol	1623.00		NIST Webbook
ripol	1602.00		NIST Webbook
tb	560.02	K	Joback Method
tc	763.29	K	Joback Method
tf	281.06	K	Joback Method
vc	0.656	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	456.30	J/molxK	560.02	Joback Method
cpg	548.42	J/molxK	729.41	Joback Method
cpg	531.98	J/molxK	695.54	Joback Method
cpg	514.55	J/molxK	661.66	Joback Method
cpg	496.13	J/molxK	627.78	Joback Method
cpg	476.71	J/molxK	593.90	Joback Method
cpg	563.88	J/molxK	763.29	Joback Method
dvisc	0.0002379	Paxs	560.02	Joback Method
dvisc	0.0003020	Paxs	513.53	Joback Method
dvisc	0.0004019	Paxs	467.03	Joback Method
dvisc	0.0005700	Paxs	420.54	Joback Method
dvisc	0.0008815	Paxs	374.05	Joback Method
dvisc	0.0015430	Paxs	327.55	Joback Method
dvisc	0.0032505	Paxs	281.06	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=U122163&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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