

Formic acid, neopentyl ester

Inchi: InChI=1S/C6H12O2/c1-6(2,3)4-8-5-7/h5H,4H2,1-3H3
InchiKey: DGMIPKNXUDSQGI-UHFFFAOYSA-N
Formula: C6H12O2
SMILES: CC(C)(C)COC=O
Mol. weight [g/mol]: 116.16

Physical Properties

Property code	Value	Unit	Source
gf	-202.04	kJ/mol	Joback Method
hf	-393.72	kJ/mol	Joback Method
hfus	7.36	kJ/mol	Joback Method
hvap	36.78	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	1.205		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	738.00		NIST Webbook
rinpol	738.00		NIST Webbook
tb	404.53	K	Joback Method
tc	588.60	K	Joback Method
tf	224.03	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.67	J/molxK	404.53	Joback Method
cpg	214.45	J/molxK	435.21	Joback Method
cpg	224.75	J/molxK	465.89	Joback Method
cpg	234.57	J/molxK	496.56	Joback Method
cpg	243.93	J/molxK	527.24	Joback Method
cpg	252.85	J/molxK	557.92	Joback Method
cpg	261.33	J/molxK	588.60	Joback Method
dvisc	0.0054671	Paxs	224.03	Joback Method

dvisc	0.0025670	Paxs	254.11	Joback Method
dvisc	0.0014145	Paxs	284.20	Joback Method
dvisc	0.0008736	Paxs	314.28	Joback Method
dvisc	0.0005870	Paxs	344.36	Joback Method
dvisc	0.0004204	Paxs	374.45	Joback Method
dvisc	0.0003164	Paxs	404.53	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=U367903&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

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