

Formic acid, 4,4-dimethylpent-2-yl ester

Inchi:	InChI=1S/C8H16O2/c1-7(10-6-9)5-8(2,3)4/h6-7H,5H2,1-4H3
InchiKey:	HDPIKLHXOVSMRM-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CC(CC(C)(C)C)OC=O
Mol. weight [g/mol]:	144.21

Physical Properties

Property code	Value	Unit	Source
gf	-187.64	kJ/mol	Joback Method
hf	-440.28	kJ/mol	Joback Method
hfus	9.02	kJ/mol	Joback Method
hvap	40.85	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.984		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	881.00		NIST Webbook
tb	449.85	K	Joback Method
tc	635.11	K	Joback Method
tf	231.57	K	Joback Method
vc	0.501	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.52	J/molxK	449.85	Joback Method
cpg	296.95	J/molxK	480.73	Joback Method
cpg	309.76	J/molxK	511.60	Joback Method
cpg	321.96	J/molxK	542.48	Joback Method
cpg	333.58	J/molxK	573.36	Joback Method
cpg	344.62	J/molxK	604.23	Joback Method
cpg	355.12	J/molxK	635.11	Joback Method
dvisc	0.0085994	Paxs	231.57	Joback Method
dvisc	0.0032553	Paxs	267.95	Joback Method

dvisc	0.0015545	Paxs	304.33	Joback Method
dvisc	0.0008692	Paxs	340.71	Joback Method
dvisc	0.0005437	Paxs	377.09	Joback Method
dvisc	0.0003694	Paxs	413.47	Joback Method
dvisc	0.0002672	Paxs	449.85	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=U368699&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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