

Acetic acid, 3-methylhept-3-yl ester

Inchi:	InChI=1S/C10H20O2/c1-5-7-8-10(4,6-2)12-9(3)11/h5-8H2,1-4H3
InchiKey:	IPSFZWUZTDNBCL-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCC(C)(CC)OC(C)=O
Mol. weight [g/mol]:	172.26

Physical Properties

Property code	Value	Unit	Source
gf	-197.76	kJ/mol	Joback Method
hf	-503.28	kJ/mol	Joback Method
hfus	17.03	kJ/mol	Joback Method
hvap	45.71	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.908		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1089.00		NIST Webbook
tb	501.26	K	Joback Method
tc	683.58	K	Joback Method
tf	277.04	K	Joback Method
vc	0.609	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.98	J/mol×K	501.26	Joback Method
cpg	386.18	J/mol×K	531.65	Joback Method
cpg	400.69	J/mol×K	562.03	Joback Method
cpg	414.52	J/mol×K	592.42	Joback Method
cpg	427.70	J/mol×K	622.81	Joback Method
cpg	440.23	J/mol×K	653.19	Joback Method
cpg	452.15	J/mol×K	683.58	Joback Method
dvisc	0.0043525	Paxs	277.04	Joback Method
dvisc	0.0019589	Paxs	314.41	Joback Method

dvisc	0.0010446	Paxs	351.78	Joback Method
dvisc	0.0006286	Paxs	389.15	Joback Method
dvisc	0.0004134	Paxs	426.52	Joback Method
dvisc	0.0002909	Paxs	463.89	Joback Method
dvisc	0.0002157	Paxs	501.26	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=U368950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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