Propanoic acid, 2,2-dimethyl-, heptyl ester

Other names: Heptyl pivalate
Inchi: InChI=1S/C12H24O2/c1-5-6-7-8-9-10-14-11(13)12(2,3)4/h5-10H2,1-4H3
InchiKey: VJQPQMJCZDBCEQ-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: CCCCCCCOC(=O)C(C)(C)C
Mol. weight [g/mol]: 200.32
CAS: 17660-61-6

Physical Properties

Property code	Value	Unit	Source
gf	-180.92	kJ/mol	Joback Method
hf	-544.56	kJ/mol	Joback Method
hfus	22.21	kJ/mol	Joback Method
hvap	50.17	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.546		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	1263.00		NIST Webbook
ripol	1428.00		NIST Webbook
tb	547.02	K	Joback Method
tc	725.77	K	Joback Method
tf	299.58	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.06	J/mol×K	547.02	Joback Method
cpg	483.65	J/mol×K	576.81	Joback Method
cpg	499.47	J/mol×K	606.60	Joback Method
cpg	514.55	J/mol×K	636.40	Joback Method
cpg	528.91	J/mol×K	666.19	Joback Method
cpg	542.58	J/mol×K	695.98	Joback Method

cpg	555.57	J/mol×K	725.77	Joback Method
dvisc	0.0038453	Pa×s	299.58	Joback Method
dvisc	0.0016806	Pa×s	340.82	Joback Method
dvisc	0.0008783	Pa×s	382.06	Joback Method
dvisc	0.0005208	Pa×s	423.30	Joback Method
dvisc	0.0003389	Pa×s	464.54	Joback Method
dvisc	0.0002365	Pa×s	505.78	Joback Method
dvisc	0.0001743	Pa×s	547.02	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17660616&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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