

2,2,4-Trimethyl-3-oxovaleric acid, 2-ethylhexyl ester

Inchi:	InChI=1S/C16H30O3/c1-7-9-10-13(8-2)11-19-15(18)16(5,6)14(17)12(3)4/h12-13H,7-11H
InchiKey:	ZNMKKKLXWORYSF-UHFFFAOYSA-N
Formula:	C16H30O3
SMILES:	CCCCC(CC)COC(=O)C(C)(C)C(=O)C(C)C
Mol. weight [g/mol]:	270.41
CAS:	4447-76-1

Physical Properties

Property code	Value	Unit	Source
gf	-281.04	kJ/mol	Joback Method
hf	-750.26	kJ/mol	Joback Method
hfus	27.12	kJ/mol	Joback Method
hvap	65.04	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.997		Crippen Method
mvol	245.310	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
tb	691.53	K	Joback Method
tc	878.10	K	Joback Method
tf	364.59	K	Joback Method
vc	0.939	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.79	J/molxK	691.53	Joback Method
cpg	786.02	J/molxK	847.00	Joback Method
cpg	771.95	J/molxK	815.91	Joback Method
cpg	757.02	J/molxK	784.81	Joback Method
cpg	741.21	J/molxK	753.72	Joback Method
cpg	724.47	J/molxK	722.62	Joback Method
cpg	799.27	J/molxK	878.10	Joback Method
dvisc	0.0000876	Paxs	691.53	Joback Method
dvisc	0.0001231	Paxs	637.04	Joback Method

dvisc	0.0001842	Paxs	582.55	Joback Method
dvisc	0.0002997	Paxs	528.06	Joback Method
dvisc	0.0005454	Paxs	473.57	Joback Method
dvisc	0.0011596	Paxs	419.08	Joback Method
dvisc	0.0030894	Paxs	364.59	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=C4447761&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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