

Hexadecanoic acid, 2,3,4-trimethyl-, methyl ester

Other names:	methyl 2,3,4-trimethylhexadecanoate
Inchi:	InChI=1S/C20H40O2/c1-6-7-8-9-10-11-12-13-14-15-16-17(2)18(3)19(4)20(21)22-5/h17-1
InchiKey:	YGOVFMOPCPODED-UHFFFAOYSA-N
Formula:	C20H40O2
SMILES:	CCCCCCCCCCCC(C)C(C)C(C)C(=O)OC
Mol. weight [g/mol]:	312.53
CAS:	55124-95-3

Physical Properties

Property code	Value	Unit	Source
gf	-123.72	kJ/mol	Joback Method
hf	-716.77	kJ/mol	Joback Method
hfus	39.77	kJ/mol	Joback Method
hvap	68.11	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	6.379		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1062.40	kPa	Joback Method
tb	731.97	K	Joback Method
tc	907.27	K	Joback Method
tf	342.32	K	Joback Method
vc	1.161	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.81	J/molxK	731.97	Joback Method
cpg	1001.13	J/molxK	878.05	Joback Method
cpg	984.73	J/molxK	848.83	Joback Method
cpg	967.43	J/molxK	819.62	Joback Method
cpg	949.19	J/molxK	790.40	Joback Method
cpg	929.99	J/molxK	761.19	Joback Method
cpg	1016.64	J/molxK	907.27	Joback Method
dvisc	0.0000576	Paxs	731.97	Joback Method

dvisc	0.0000823	Paxs	667.03	Joback Method
dvisc	0.0001268	Paxs	602.09	Joback Method
dvisc	0.0002170	Paxs	537.14	Joback Method
dvisc	0.0004305	Paxs	472.20	Joback Method
dvisc	0.0010626	Paxs	407.26	Joback Method
dvisc	0.0036948	Paxs	342.32	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C55124953&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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