

Hexanoic acid, 2-ethyl-, methyl ester

Other names:	Methyl 2-ethylhexanoate Methyl ester of 2-ethylhexanoic acid
Inchi:	InChI=1S/C9H18O2/c1-4-6-7-8(5-2)9(10)11-3/h8H,4-7H2,1-3H3
InchiKey:	KICUISADAVMYCJ-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCC(CC)C(=O)OC
Mol. weight [g/mol]:	158.24
CAS:	816-19-3

Physical Properties

Property code	Value	Unit	Source
gf	-211.46	kJ/mol	Joback Method
hf	-479.17	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	44.40	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.376		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1043.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1031.00		NIST Webbook
tb	481.17	K	Joback Method
tc	658.49	K	Joback Method
tf	248.35	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.06	J/molxK	481.17	Joback Method
cpg	336.66	J/molxK	510.72	Joback Method
cpg	349.76	J/molxK	540.28	Joback Method

cpg	362.35	J/molxK	569.83	Joback Method
cpg	374.44	J/molxK	599.38	Joback Method
cpg	386.04	J/molxK	628.93	Joback Method
cpg	397.15	J/molxK	658.49	Joback Method
dvisc	0.0047844	Paxs	248.35	Joback Method
dvisc	0.0020429	Paxs	287.15	Joback Method
dvisc	0.0010682	Paxs	325.96	Joback Method
dvisc	0.0006412	Paxs	364.76	Joback Method
dvisc	0.0004246	Paxs	403.56	Joback Method
dvisc	0.0003022	Paxs	442.37	Joback Method
dvisc	0.0002272	Paxs	481.17	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=C816193&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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