

2-Ethylbutyric acid, 3,7-dimethyloctyl ester

Inchi:	InChI=1S/C16H32O2/c1-6-15(7-2)16(17)18-12-11-14(5)10-8-9-13(3)4/h13-15H,6-12H2,1
InchiKey:	XIEJABOHANHRAF-UHFFFAOYSA-N
Formula:	C16H32O2
SMILES:	CCC(CC)C(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]:	256.42

Physical Properties

Property code	Value	Unit	Source
gf	-157.40	kJ/mol	Joback Method
hf	-634.21	kJ/mol	Joback Method
hfus	29.41	kJ/mol	Joback Method
hvap	59.20	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.818		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1388.15	kPa	Joback Method
rinsol	1564.00		NIST Webbook
tb	640.45	K	Joback Method
tc	814.89	K	Joback Method
tf	297.24	K	Joback Method
vc	0.938	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.98	J/molxK	640.45	Joback Method
cpg	695.74	J/molxK	669.52	Joback Method
cpg	713.66	J/molxK	698.60	Joback Method
cpg	730.76	J/molxK	727.67	Joback Method
cpg	747.04	J/molxK	756.74	Joback Method
cpg	762.54	J/molxK	785.82	Joback Method
cpg	777.26	J/molxK	814.89	Joback Method
dvisc	0.0061918	Paxs	297.24	Joback Method
dvisc	0.0017774	Paxs	354.44	Joback Method

dvisc	0.0007217	Paxs	411.64	Joback Method
dvisc	0.0003652	Paxs	468.85	Joback Method
dvisc	0.0002143	Paxs	526.05	Joback Method
dvisc	0.0001396	Paxs	583.25	Joback Method
dvisc	0.0000982	Paxs	640.45	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=U369419&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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