

2-Ethylbutyric acid, 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C14H28O2/c1-7-12(8-2)13(15)16-10-11(3)9-14(4,5)6/h11-12H,7-10H2,1-6H3
InchiKey:	WLQKSHVRTDKBAH-UHFFFAOYSA-N
Formula:	C14H28O2
SMILES:	CCC(CC)C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	228.37

Physical Properties

Property code	Value	Unit	Source
gf	-168.96	kJ/mol	Joback Method
hf	-596.40	kJ/mol	Joback Method
hfus	20.34	kJ/mol	Joback Method
hvap	53.84	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	4.038		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpola	1320.00		NIST Webbook
tb	591.90	K	Joback Method
tc	773.91	K	Joback Method
tf	292.12	K	Joback Method
vc	0.821	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.41	J/molxK	591.90	Joback Method
cpg	588.77	J/molxK	622.23	Joback Method
cpg	606.24	J/molxK	652.57	Joback Method
cpg	622.85	J/molxK	682.90	Joback Method
cpg	638.63	J/molxK	713.24	Joback Method
cpg	653.60	J/molxK	743.57	Joback Method
cpg	667.79	J/molxK	773.91	Joback Method
dvisc	0.0066207	Paxs	292.12	Joback Method
dvisc	0.0020827	Paxs	342.08	Joback Method

dvisc	0.0008798	Paxs	392.05	Joback Method
dvisc	0.0004516	Paxs	442.01	Joback Method
dvisc	0.0002654	Paxs	491.97	Joback Method
dvisc	0.0001721	Paxs	541.94	Joback Method
dvisc	0.0001200	Paxs	591.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369493&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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