

2-Ethylbutyric acid, cyclohexylmethyl ester

Inchi:	InChI=1S/C13H24O2/c1-3-12(4-2)13(14)15-10-11-8-6-5-7-9-11/h11-12H,3-10H2,1-2H3
InchiKey:	AXBLNGFHTFZDPG-UHFFFAOYSA-N
Formula:	C13H24O2
SMILES:	CCC(CC)C(=O)OCC1CCCCC1
Mol. weight [g/mol]:	212.33

Physical Properties

Property code	Value	Unit	Source
gf	-153.33	kJ/mol	Joback Method
hf	-507.41	kJ/mol	Joback Method
hfus	20.52	kJ/mol	Joback Method
hvap	53.73	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.546		Crippen Method
mcvol	190.610	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinqol	1470.00		NIST Webbook
tb	592.24	K	Joback Method
tc	792.82	K	Joback Method
tf	300.81	K	Joback Method
vc	0.715	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.82	J/molxK	592.24	Joback Method
cpg	526.80	J/molxK	625.67	Joback Method
cpg	545.72	J/molxK	659.10	Joback Method
cpg	563.61	J/molxK	692.53	Joback Method
cpg	580.48	J/molxK	725.96	Joback Method
cpg	596.36	J/molxK	759.39	Joback Method
cpg	611.27	J/molxK	792.82	Joback Method
dvisc	0.0049796	Paxs	300.81	Joback Method
dvisc	0.0019175	Paxs	349.38	Joback Method

dvisc	0.0009321	Paxs	397.95	Joback Method
dvisc	0.0005301	Paxs	446.52	Joback Method
dvisc	0.0003368	Paxs	495.10	Joback Method
dvisc	0.0002320	Paxs	543.67	Joback Method
dvisc	0.0001699	Paxs	592.24	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=U357752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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