

Cyclohexaneacetic acid, «alpha»-ethyl-

Other names:	2-Cyclohexyl-n-butyric acid 2-Cyclohexylbutanoic acid «alpha»-Ethylcyclohexaneacetic acid Alpha-ethylcyclohexaneacetic acid 2-cyclohexylbutyric acid
Inchi:	InChI=1S/C10H18O2/c1-2-9(10(11)12)8-6-4-3-5-7-8/h8-9H,2-7H2,1H3,(H,11,12)
InchiKey:	RPXFDOOFVNTCQA-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CCC(C(=O)O)C1CCCCC1
Mol. weight [g/mol]:	170.25
CAS:	6051-00-9

Physical Properties

Property code	Value	Unit	Source
gf	-210.41	kJ/mol	Joback Method
hf	-465.50	kJ/mol	Joback Method
hfus	15.65	kJ/mol	Joback Method
hvap	61.32	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.678		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
tb	593.36	K	Joback Method
tc	791.33	K	Joback Method
tf	305.59	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.30	J/mol×K	593.36	Joback Method
cpg	407.73	J/mol×K	626.35	Joback Method
cpg	422.30	J/mol×K	659.35	Joback Method
cpg	436.03	J/mol×K	692.34	Joback Method

cpg	448.96	J/mol×K	725.34	Joback Method
cpg	461.10	J/mol×K	758.33	Joback Method
cpg	472.49	J/mol×K	791.33	Joback Method
dvisc	0.0206210	Pa×s	305.59	Joback Method
dvisc	0.0045993	Pa×s	353.55	Joback Method
dvisc	0.0014681	Pa×s	401.51	Joback Method
dvisc	0.0005979	Pa×s	449.47	Joback Method
dvisc	0.0002896	Pa×s	497.44	Joback Method
dvisc	0.0001593	Pa×s	545.40	Joback Method
dvisc	0.0000965	Pa×s	593.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6051009&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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