Cyclohexanecarboxylic acid, hexyl ester

Other names: hexyl cyclohexanecarboxylate
Inchi: InChI=1S/C13H24O2/c1-2-3-4-8-11-15-13(14)12-9-6-5-7-10-12/h12H,2-11H2,1H3
InchiKey: QNVYTFRSSXVBQH-UHFFFAOYSA-N
Formula: C13H24O2
SMILES: CCCCCCOC(=O)C1CCCCC1
Mol. weight [g/mol]: 212.33
CAS: 27948-10-3

Physical Properties

Property code	Value	Unit	Source
gf	-150.89	kJ/mol	Joback Method
hf	-502.13	kJ/mol	Joback Method
hfus	24.05	kJ/mol	Joback Method
hvap	54.12	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.690		Crippen Method
mcvol	190.610	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1506.12		NIST Webbook
rinpol	1506.12		NIST Webbook
rinpol	1509.71		NIST Webbook
tb	592.68	K	Joback Method
tc	789.39	K	Joback Method
tf	315.81	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.49	J/mol×K	592.68	Joback Method
cpg	526.03	J/mol×K	625.46	Joback Method
cpg	544.57	J/mol×K	658.25	Joback Method
cpg	562.11	J/mol×K	691.03	Joback Method
cpg	578.69	J/mol×K	723.82	Joback Method

cpg	594.33	J/mol×K	756.60	Joback Method
cpg	609.03	J/mol×K	789.39	Joback Method
dvisc	0.0036457	Pa×s	315.81	Joback Method
dvisc	0.0016084	Pa×s	361.95	Joback Method
dvisc	0.0008539	Pa×s	408.10	Joback Method
dvisc	0.0005155	Pa×s	454.25	Joback Method
dvisc	0.0003416	Pa×s	500.39	Joback Method
dvisc	0.0002426	Pa×s	546.53	Joback Method
dvisc	0.0001818	Pa×s	592.68	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=C27948103&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