Cyclohexane, 1-hexylcarbonyl-4-(1,1-dimethylethyl), # 1

Inchi: InChI=1S/C17H32O/c1-5-6-7-8-9-16(18)14-10-12-15(13-11-14)17(2,3)4/h14-15H,5-13H2

InchiKey: SCAVUHKXZBPJLH-UHFFFAOYSA-N

Formula: C17H32O

SMILES: CCCCCCC(=O)C1CCC(C(C)(C)C)CC1

Mol. weight [g/mol]: 252.44

Physical Properties

Property code	Value	Unit	Source
gf	-17.08	kJ/mol	Joback Method
hf	-481.56	kJ/mol	Joback Method
hfus	26.88	kJ/mol	Joback Method
hvap	59.01	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	5.378		Crippen Method
mcvol	241.100	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1784.00		NIST Webbook
ripol	2187.00		NIST Webbook
ripol	2187.00		NIST Webbook
ripol	2267.00		NIST Webbook
ripol	2227.00		NIST Webbook
tb	653.88	K	Joback Method
tc	852.18	K	Joback Method
tf	336.84	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.83	J/mol×K	653.88	Joback Method
cpg	722.37	J/mol×K	686.93	Joback Method

cpg	743.62	J/mol×K	719.98	Joback Method
cpg	763.61	J/mol×K	753.03	Joback Method
cpg	782.41	J/mol×K	786.08	Joback Method
cpg	800.06	J/mol×K	819.13	Joback Method
cpg	816.61	J/mol×K	852.18	Joback Method
dvisc	0.0039961	Pa×s	336.84	Joback Method
dvisc	0.0015995	Pa×s	389.68	Joback Method
dvisc	0.0007967	Pa×s	442.52	Joback Method
dvisc	0.0004605	Pa×s	495.36	Joback Method
dvisc	0.0002958	Pa×s	548.20	Joback Method
dvisc	0.0002054	Pa×s	601.04	Joback Method
dvisc	0.0001513	Pa×s	653.88	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R97755&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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume