1,2-Cyclohexanedicarboxylic acid, isobutyl propyl ester

Inchi: InChI=1S/C15H26O4/c1-4-9-18-14(16)12-7-5-6-8-13(12)15(17)19-10-11(2)3/h11-13H,4-1

InchiKey: SZAJLQTUDWVUSQ-UHFFFAOYSA-N

Formula: C15H26O4

SMILES: CCCOC(=O)C1CCCCC1C(=O)OCC(C)C

Mol. weight [g/mol]: 270.36

Physical Properties

Property code	Value	Unit	Source
gf	-378.12	kJ/mol	Joback Method
hf	-813.83	kJ/mol	Joback Method
hfus	29.56	kJ/mol	Joback Method
hvap	67.03	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.945		Crippen Method
mcvol	226.230	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	1790.00		NIST Webbook
rinpol	1790.00		NIST Webbook
tb	709.62	K	Joback Method
tc	910.33	K	Joback Method
tf	391.27	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.70	J/mol×K	709.62	Joback Method
cpg	757.63	J/mol×K	876.88	Joback Method
cpg	743.34	J/mol×K	843.43	Joback Method
cpg	727.90	J/mol×K	809.98	Joback Method
cpg	711.32	J/mol×K	776.52	Joback Method
cpg	693.58	J/mol×K	743.07	Joback Method
cpg	770.79	J/mol×K	910.33	Joback Method
dvisc	0.0001251	Pa×s	709.62	Joback Method

dvisc	0.0001640	Pa×s	656.56	Joback Method
dvisc	0.0002254	Pa×s	603.50	Joback Method
dvisc	0.0003292	Pa×s	550.44	Joback Method
dvisc	0.0005216	Pa×s	497.39	Joback Method
dvisc	0.0009222	Pa×s	444.33	Joback Method
dvisc	0.0019030	Pa×s	391.27	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=U339423&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

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