1,2-Cyclohexanedicarboxylic acid, cyclobutyl hexyl ester

Inchi: InChI=1S/C18H30O4/c1-2-3-4-7-13-21-17(19)15-11-5-6-12-16(15)18(20)22-14-9-8-10-14

InchiKey: ZEJUBRIRNHIJNG-UHFFFAOYSA-N

Formula: C18H30O4

SMILES: CCCCCCOC(=O)C1CCCCC1C(=O)OC1CCC1

Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-301.77	kJ/mol	Joback Method
hf	-803.83	kJ/mol	Joback Method
hfus	36.89	kJ/mol	Joback Method
hvap	74.18	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.012		Crippen Method
mcvol	257.640	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
rinpol	2257.00		NIST Webbook
rinpol	2257.00		NIST Webbook
tb	789.71	K	Joback Method
tc	997.19	K	Joback Method
tf	454.50	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.38	J/mol×K	789.71	Joback Method
cpg	922.22	J/mol×K	962.61	Joback Method
cpg	907.92	J/mol×K	928.03	Joback Method
cpg	892.31	J/mol×K	893.45	Joback Method
cpg	875.38	J/mol×K	858.87	Joback Method
cpg	857.08	J/mol×K	824.29	Joback Method
cpg	935.25	J/mol×K	997.19	Joback Method
dvisc	0.0001935	Pa×s	789.71	Joback Method

dvisc	0.0002419	Pa×s	733.84	Joback Method
dvisc	0.0003137	Pa×s	677.97	Joback Method
dvisc	0.0004264	Pa×s	622.11	Joback Method
dvisc	0.0006156	Pa×s	566.24	Joback Method
dvisc	0.0009633	Pa×s	510.37	Joback Method
dvisc	0.0016827	Pa×s	454.50	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=U339752&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