1,2-Cyclohexanedicarboxylic acid, heptyl octyl ester

Inchi: InChI=1S/C23H42O4/c1-3-5-7-9-11-15-19-27-23(25)21-17-13-12-16-20(21)22(24)26-18-

InchiKey: STURPVSRWWYUMZ-UHFFFAOYSA-N

Formula: C23H42O4

SMILES: CCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCCCCC

Mol. weight [g/mol]: 382.58

Physical Properties

Property code	Value	Unit	Source
gf	-308.32	kJ/mol	Joback Method
hf	-973.67	kJ/mol	Joback Method
hfus	53.81	kJ/mol	Joback Method
hvap	85.22	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	6.210		Crippen Method
mcvol	338.950	ml/mol	McGowan Method
pc	1000.18	kPa	Joback Method
rinpol	2623.00		NIST Webbook
rinpol	2623.00		NIST Webbook
tb	893.10	K	Joback Method
tc	1095.01	K	Joback Method
tf	496.43	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.63	J/mol×K	893.10	Joback Method
cpg	1175.24	J/mol×K	926.75	Joback Method
cpg	1193.32	J/mol×K	960.40	Joback Method
cpg	1209.91	J/mol×K	994.05	Joback Method
cpg	1225.04	J/mol×K	1027.71	Joback Method
cpg	1238.73	J/mol×K	1061.36	Joback Method
cpg	1251.01	J/mol×K	1095.01	Joback Method
dvisc	0.0007325	Pa×s	496.43	Joback Method

dvisc	0.0003525	Pa×s	562.54	Joback Method
dvisc	0.0001979	Pa×s	628.65	Joback Method
dvisc	0.0001240	Pa×s	694.76	Joback Method
dvisc	0.0000842	Pa×s	760.88	Joback Method
dvisc	0.0000609	Pa×s	826.99	Joback Method
dvisc	0.0000462	Pa×s	893.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339539&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume