1,2-Cyclohexanedicarboxylic acid, 2-cyclohexylethyl heptyl ester

Inchi: InChI=1S/C23H40O4/c1-2-3-4-5-11-17-26-22(24)20-14-9-10-15-21(20)23(25)27-18-16-1

InchiKey: WVUPCHNXKOTUKJ-UHFFFAOYSA-N

Formula: C23H40O4

SMILES: CCCCCCCOC(=O)C1CCCCC1C(=O)OCCC1CCCCC1

Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-283.87	kJ/mol	Joback Method
hf	-919.35	kJ/mol	Joback Method
hfus	45.64	kJ/mol	Joback Method
hvap	85.65	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.820		Crippen Method
mcvol	328.090	ml/mol	McGowan Method
pc	1143.66	kPa	Joback Method
rinpol	2699.00		NIST Webbook
rinpol	2699.00		NIST Webbook
tb	912.65	K	Joback Method
tc	1126.39	K	Joback Method
tf	503.81	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.85	J/mol×K	912.65	Joback Method
cpg	1233.18	J/mol×K	1090.76	Joback Method
cpg	1220.61	J/mol×K	1055.14	Joback Method
cpg	1206.33	J/mol×K	1019.52	Joback Method
cpg	1190.30	J/mol×K	983.90	Joback Method
cpg	1172.48	J/mol×K	948.27	Joback Method
cpg	1244.06	J/mol×K	1126.39	Joback Method
dvisc	0.0000477	Pa×s	912.65	Joback Method

dvisc	0.0000633	Pa×s	844.51	Joback Method
dvisc	0.0000884	Pa×s	776.37	Joback Method
dvisc	0.0001317	Pa×s	708.23	Joback Method
dvisc	0.0002135	Pa×s	640.09	Joback Method
dvisc	0.0003883	Pa×s	571.95	Joback Method
dvisc	0.0008302	Pa×s	503.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339728&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume