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

Inchi: InChI=1S/C20H36O4/c1-4-6-7-8-11-14-23-19(21)17-12-9-10-13-18(17)20(22)24-15-16(3
InchiKey: IEIFHCNXAFLDNG-UHFFFAOYSA-N
Formula: C20H36O4
SMILES: CCCCCCCOC(=O)C1CCCCC1C(=O)OCC(C)CC
Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-336.02	kJ/mol	Joback Method
hf	-917.03	kJ/mol	Joback Method
hfus	42.51	kJ/mol	Joback Method
hvap	78.16	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.896		Crippen Method
mcvol	296.680	ml/mol	McGowan Method
pc	1217.44	kPa	Joback Method
rinpol	2274.00		NIST Webbook
rinpol	2274.00		NIST Webbook
tb	824.02	K	Joback Method
tc	1020.98	K	Joback Method
tf	447.62	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.98	J/mol×K	824.02	Joback Method
cpg	989.40	J/mol×K	856.85	Joback Method
cpg	1007.46	J/mol×K	889.67	Joback Method
cpg	1024.18	J/mol×K	922.50	Joback Method
cpg	1039.58	J/mol×K	955.33	Joback Method
cpg	1053.69	J/mol×K	988.16	Joback Method
cpg	1066.50	J/mol×K	1020.98	Joback Method
dvisc	0.0011819	Pa×s	447.62	Joback Method

dvisc	0.0005412	Pa×s	510.35	Joback Method
dvisc	0.0002940	Pa×s	573.09	Joback Method
dvisc	0.0001802	Pa×s	635.82	Joback Method
dvisc	0.0001206	Pa×s	698.55	Joback Method
dvisc	0.0000862	Pa×s	761.29	Joback Method
dvisc	0.0000648	Pa×s	824.02	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=U339547&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