cis-Cyclohex-4-en-1,2-dicarboxylic acid, isohexyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C20H34O4/c1-6-18(15(4)5)24-20(22)17-12-8-7-11-16(17)19(21)23-13-9-10-14

InchiKey: HUSDHEKLRDEXEN-UHFFFAOYSA-N

Formula: C20H34O4

SMILES: CCC(OC(=O)C1CC=CCC1C(=O)OCCCC(C)C)C(C)C

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-310.94	kJ/mol	Joback Method
hf	-869.81	kJ/mol	Joback Method
hfus	36.69	kJ/mol	Joback Method
hvap	77.67	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.526		Crippen Method
mcvol	292.380	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
rinpol	2198.00		NIST Webbook
tb	822.30	K	Joback Method
tc	1023.83	K	Joback Method
tf	418.38	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.09	J/mol×K	822.30	Joback Method
cpg	1024.53	J/mol×K	990.24	Joback Method
cpg	1010.93	J/mol×K	956.65	Joback Method
cpg	996.01	J/mol×K	923.06	Joback Method
cpg	979.74	J/mol×K	889.48	Joback Method
cpg	962.11	J/mol×K	855.89	Joback Method
cpg	1036.82	J/mol×K	1023.83	Joback Method
dvisc	0.0000587	Pa×s	822.30	Joback Method
dvisc	0.0000798	Pa×s	754.98	Joback Method

dvisc	0.0001151	Pa×s	687.66	Joback Method
dvisc	0.0001797	Pa×s	620.34	Joback Method
dvisc	0.0003127	Pa×s	553.02	Joback Method
dvisc	0.0006348	Pa×s	485.70	Joback Method
dvisc	0.0016181	Pa×s	418.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382762&Units=SI

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