1,2-Cyclohexanedicarboxylic acid, heptyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C21H38O4/c1-5-7-8-9-12-15-24-20(22)17-13-10-11-14-18(17)21(23)25-19(6-2
InchiKey: FANMCFKLQGEBMK-UHFFFAOYSA-N
Formula: C21H38O4
SMILES: CCCCCCCOC(=O)C1CCCCC1C(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-330.04	kJ/mol	Joback Method
hf	-942.95	kJ/mol	Joback Method
hfus	41.58	kJ/mol	Joback Method
hvap	80.00	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.284		Crippen Method
mcvol	310.770	ml/mol	McGowan Method
pc	1145.99	kPa	Joback Method
rinpol	2369.00		NIST Webbook
rinpol	2369.00		NIST Webbook
tb	846.46	K	Joback Method
tc	1046.00	K	Joback Method
tf	443.89	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.88	J/mol×K	846.46	Joback Method
cpg	1051.50	J/mol×K	879.72	Joback Method
cpg	1069.67	J/mol×K	912.97	Joback Method
cpg	1086.43	J/mol×K	946.23	Joback Method
cpg	1101.80	J/mol×K	979.48	Joback Method
cpg	1115.78	J/mol×K	1012.74	Joback Method
cpg	1128.41	J/mol×K	1046.00	Joback Method
dvisc	0.0012526	Pa×s	443.89	Joback Method

dvisc	0.0005193	Pa×s	510.99	Joback Method
dvisc	0.0002641	Pa×s	578.08	Joback Method
dvisc	0.0001546	Pa×s	645.17	Joback Method
dvisc	0.0001001	Pa×s	712.27	Joback Method
dvisc	0.0000699	Pa×s	779.37	Joback Method
dvisc	0.0000516	Pa×s	846.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339444&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