1,2-Cyclohexanedicarboxylic acid, decyl isobutyl ester

Inchi: InChI=1S/C22H40O4/c1-4-5-6-7-8-9-10-13-16-25-21(23)19-14-11-12-15-20(19)22(24)26
InchiKey: XTLZHMNYSDYCTM-UHFFFAOYSA-N
Formula: C22H40O4
SMILES: CCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-319.18	kJ/mol	Joback Method
hf	-958.31	kJ/mol	Joback Method
hfus	47.69	kJ/mol	Joback Method
hvap	82.61	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.676		Crippen Method
mcvol	324.860	ml/mol	McGowan Method
pc	1069.36	kPa	Joback Method
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook
tb	869.78	K	Joback Method
tc	1069.70	K	Joback Method
tf	470.16	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.46	J/mol×K	869.78	Joback Method
cpg	1176.80	J/mol×K	1036.38	Joback Method
cpg	1162.98	J/mol×K	1003.06	Joback Method
cpg	1147.76	J/mol×K	969.74	Joback Method
cpg	1131.11	J/mol×K	936.42	Joback Method
cpg	1113.02	J/mol×K	903.10	Joback Method
cpg	1189.25	J/mol×K	1069.70	Joback Method
dvisc	0.0000488	Pa×s	869.78	Joback Method

dvisc	0.0000652	Pa×s	803.18	Joback Method
dvisc	0.0000917	Pa×s	736.57	Joback Method
dvisc	0.0001381	Pa×s	669.97	Joback Method
dvisc	0.0002276	Pa×s	603.37	Joback Method
dvisc	0.0004247	Pa×s	536.76	Joback Method
dvisc	0.0009457	Pa×s	470.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339431&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