

1,2-Cyclohexanedicarboxylic acid, decyl hexyl ester

Inchi:	InChI=1S/C24H44O4/c1-3-5-7-9-10-11-12-16-20-28-24(26)22-18-14-13-17-21(22)23(25)
InchiKey:	VXCYTMDMIPWIKM-UHFFFAOYSA-N
Formula:	C24H44O4
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCCC
Mol. weight [g/mol]:	396.60

Physical Properties

Property code	Value	Unit	Source
gf	-299.90	kJ/mol	Joback Method
hf	-994.31	kJ/mol	Joback Method
hfus	56.40	kJ/mol	Joback Method
hvap	87.45	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.600		Crippen Method
mcvol	353.040	ml/mol	McGowan Method
pc	942.10	kPa	Joback Method
rinsol	2717.00		NIST Webbook
tb	915.98	K	Joback Method
tc	1121.76	K	Joback Method
tf	507.70	K	Joback Method
vc	1.359	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.74	J/molxK	915.98	Joback Method
cpg	1238.49	J/molxK	950.28	Joback Method
cpg	1256.64	J/molxK	984.57	Joback Method
cpg	1273.21	J/molxK	1018.87	Joback Method
cpg	1288.23	J/molxK	1053.16	Joback Method
cpg	1301.75	J/molxK	1087.46	Joback Method
cpg	1313.78	J/molxK	1121.76	Joback Method
dvisc	0.0006525	Paxs	507.70	Joback Method
dvisc	0.0003110	Paxs	575.75	Joback Method

dvisc	0.0001733	Paxs	643.79	Joback Method
dvisc	0.0001080	Paxs	711.84	Joback Method
dvisc	0.0000731	Paxs	779.89	Joback Method
dvisc	0.0000527	Paxs	847.93	Joback Method
dvisc	0.0000399	Paxs	915.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339415&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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