

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

Inchi:	InChI=1S/C24H44O4/c1-5-7-8-9-10-11-12-15-18-27-23(25)20-16-13-14-17-21(20)24(26)
InchiKey:	OGWABIQCALVKOP-UHFFFAOYSA-N
Formula:	C24H44O4
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	396.60

Physical Properties

Property code	Value	Unit	Source
gf	-304.78	kJ/mol	Joback Method
hf	-1004.87	kJ/mol	Joback Method
hfus	49.35	kJ/mol	Joback Method
hvap	86.67	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.454		Crippen Method
mvol	353.040	ml/mol	McGowan Method
pc	951.42	kPa	Joback Method
rinpol	2670.00		NIST Webbook
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tb	915.10	K	Joback Method
tc	1121.60	K	Joback Method
tf	477.70	K	Joback Method
vc	1.347	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1219.56	J/molxK	915.10	Joback Method
cpg	1302.30	J/molxK	1087.18	Joback Method
cpg	1288.91	J/molxK	1052.77	Joback Method
cpg	1273.97	J/molxK	1018.35	Joback Method
cpg	1257.45	J/molxK	983.93	Joback Method
cpg	1239.32	J/molxK	949.52	Joback Method
cpg	1314.18	J/molxK	1121.60	Joback Method
dvisc	0.0000332	Paxs	915.10	Joback Method

dvisc	0.0000452	Paxs	842.20	Joback Method
dvisc	0.0000653	Paxs	769.30	Joback Method
dvisc	0.0001017	Paxs	696.40	Joback Method
dvisc	0.0001758	Paxs	623.50	Joback Method
dvisc	0.0003513	Paxs	550.60	Joback Method
dvisc	0.0008669	Paxs	477.70	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=U339447&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

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