

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

Inchi:	InChI=1S/C23H40O4/c1-5-7-8-9-10-11-14-17-26-22(24)19-15-12-13-16-20(19)23(25)27-
InchiKey:	KBYJXEYLFUSFEA-UHFFFAOYSA-N
Formula:	C23H40O4
SMILES:	CCCCCCCCCOC(=O)C1CC=CCC1C(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	380.56

Physical Properties

Property code	Value	Unit	Source
gf	-283.24	kJ/mol	Joback Method
hf	-926.45	kJ/mol	Joback Method
hfus	47.98	kJ/mol	Joback Method
hvap	84.74	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.840		Crippen Method
mvol	334.650	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
rinpol	2533.00		NIST Webbook
rinpol	2533.00		NIST Webbook
tb	891.38	K	Joback Method
tc	1095.04	K	Joback Method
tf	467.19	K	Joback Method
vc	1.278	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.93	J/molxK	891.38	Joback Method
cpg	1207.13	J/molxK	1061.09	Joback Method
cpg	1194.00	J/molxK	1027.15	Joback Method
cpg	1179.44	J/molxK	993.21	Joback Method
cpg	1163.43	J/molxK	959.27	Joback Method
cpg	1145.94	J/molxK	925.32	Joback Method
cpg	1218.86	J/molxK	1095.04	Joback Method
dvisc	0.0000419	Paxs	891.38	Joback Method

dvisc	0.0000564	Paxs	820.68	Joback Method
dvisc	0.0000802	Paxs	749.98	Joback Method
dvisc	0.0001228	Paxs	679.28	Joback Method
dvisc	0.0002075	Paxs	608.59	Joback Method
dvisc	0.0004027	Paxs	537.89	Joback Method
dvisc	0.0009548	Paxs	467.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382766&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
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

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