

1,2-Cyclohexanedicarboxylic acid, di(3,5-dimethylcyclohexyl) ester

Inchi:	InChI=1S/C24H40O4/c1-15-9-16(2)12-19(11-15)27-23(25)21-7-5-6-8-22(21)24(26)28-20
InchiKey:	WTHSTRVGZOYERL-UHFFFAOYSA-N
Formula:	C24H40O4
SMILES:	CC1CC(C)CC(OC(=O)C2CCCCC2C(=O)OC2CC(C)CC(C)C2)C1
Mol. weight [g/mol]:	392.57

Physical Properties

Property code	Value	Unit	Source
gf	-281.84	kJ/mol	Joback Method
hf	-967.03	kJ/mol	Joback Method
hfus	44.35	kJ/mol	Joback Method
hvap	87.07	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.529		Crippen Method
mvol	331.320	ml/mol	McGowan Method
pc	1126.08	kPa	Joback Method
rinpol	2657.00		NIST Webbook
tb	936.40	K	Joback Method
tc	1166.61	K	Joback Method
tf	505.50	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1228.10	J/molxK	936.40	Joback Method
cpg	1305.84	J/molxK	1128.24	Joback Method
cpg	1295.47	J/molxK	1089.87	Joback Method
cpg	1282.52	J/molxK	1051.50	Joback Method
cpg	1266.99	J/molxK	1013.14	Joback Method
cpg	1248.85	J/molxK	974.77	Joback Method
cpg	1313.65	J/molxK	1166.61	Joback Method
dvisc	0.0001307	Paxs	936.40	Joback Method
dvisc	0.0001624	Paxs	864.58	Joback Method

dvisc	0.0002097	Paxs	792.77	Joback Method
dvisc	0.0002850	Paxs	720.95	Joback Method
dvisc	0.0004145	Paxs	649.13	Joback Method
dvisc	0.0006617	Paxs	577.32	Joback Method
dvisc	0.0012066	Paxs	505.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339857&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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