1,2-Cyclohexanedicarboxylic acid, 3,5-dimethylcyclohexyl nonyl ester

Inchi: InChI=1S/C25H44O4/c1-4-5-6-7-8-9-12-15-28-24(26)22-13-10-11-14-23(22)25(27)29-21
InchiKey: QUDRMGFSMXKFSN-UHFFFAOYSA-N
Formula: C25H44O4
SMILES: CCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1CC(C)CC(C)C1
Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-282.45	kJ/mol	Joback Method
hf	-1001.31	kJ/mol	Joback Method
hfus	52.96	kJ/mol	Joback Method
hvap	89.49	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	6.454		Crippen Method
mcvol	356.270	ml/mol	McGowan Method
pc	967.47	kPa	Joback Method
rinpol	2760.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	949.07	K	Joback Method
tc	1165.27	K	Joback Method
tf	517.87	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1286.96	J/mol×K	949.07	Joback Method
cpg	1365.28	J/mol×K	1129.24	Joback Method
cpg	1353.65	J/mol×K	1093.20	Joback Method
cpg	1340.03	J/mol×K	1057.17	Joback Method
cpg	1324.39	J/mol×K	1021.14	Joback Method
cpg	1306.71	J/mol×K	985.10	Joback Method
cpg	1374.94	J/mol×K	1165.27	Joback Method
dvisc	0.0000626	Pa×s	949.07	Joback Method

dvisc	0.0000805	Pa×s	877.20	Joback Method
dvisc	0.0001081	Pa×s	805.34	Joback Method
dvisc	0.0001540	Pa×s	733.47	Joback Method
dvisc	0.0002368	Pa×s	661.60	Joback Method
dvisc	0.0004045	Pa×s	589.74	Joback Method
dvisc	0.0008016	Pa×s	517.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339851&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