

Glutaric acid, di(3,5-dimethylcyclohexyl) ester

Inchi:	InChI=1S/C21H36O4/c1-14-8-15(2)11-18(10-14)24-20(22)6-5-7-21(23)25-19-12-16(3)9-
InchiKey:	SSMLRCVHYKFROE-UHFFFAOYSA-N
Formula:	C21H36O4
SMILES:	CC1CC(C)CC(OC(=O)CCCC(=O)OC2CC(C)CC(C)C2)C1
Mol. weight [g/mol]:	352.51

Physical Properties

Property code	Value	Unit	Source
gf	-323.84	kJ/mol	Joback Method
hf	-939.09	kJ/mol	Joback Method
hfus	43.67	kJ/mol	Joback Method
hvap	80.27	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.893		Crippen Method
mcvol	299.910	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
rinqol	2378.00		NIST Webbook
tb	852.88	K	Joback Method
tc	1065.06	K	Joback Method
tf	468.55	K	Joback Method
vc	1.121	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.35	J/molxK	852.88	Joback Method
cpg	1059.64	J/molxK	888.24	Joback Method
cpg	1079.05	J/molxK	923.61	Joback Method
cpg	1096.57	J/molxK	958.97	Joback Method
cpg	1112.23	J/molxK	994.34	Joback Method
cpg	1126.01	J/molxK	1029.70	Joback Method
cpg	1137.93	J/molxK	1065.06	Joback Method
dvisc	0.0012392	Paxs	468.55	Joback Method
dvisc	0.0006898	Paxs	532.61	Joback Method

dvisc	0.0004355	Paxs	596.66	Joback Method
dvisc	0.0003006	Paxs	660.71	Joback Method
dvisc	0.0002215	Paxs	724.77	Joback Method
dvisc	0.0001715	Paxs	788.83	Joback Method
dvisc	0.0001380	Paxs	852.88	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=U405410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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