

Glutaric acid, cyclohexylmethyl decyl ester

Inchi: InChI=1S/C22H40O4/c1-2-3-4-5-6-7-8-12-18-25-21(23)16-13-17-22(24)26-19-20-14-10-9
InchiKey: KTLBXVITVGDWBF-UHFFFAOYSA-N
Formula: C22H40O4
SMILES: CCCCCCCCCOC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-309.03	kJ/mol	Joback Method
hf	-932.69	kJ/mol	Joback Method
hfus	50.14	kJ/mol	Joback Method
hvap	83.31	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.964		Crippen Method
mcvol	324.860	ml/mol	McGowan Method
pc	1087.06	kPa	Joback Method
rinpol	2671.00		NIST Webbook
tb	874.89	K	Joback Method
tc	1074.52	K	Joback Method
tf	489.40	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.55	J/molxK	874.89	Joback Method
cpg	1108.72	J/molxK	908.16	Joback Method
cpg	1126.49	J/molxK	941.43	Joback Method
cpg	1142.88	J/molxK	974.70	Joback Method
cpg	1157.93	J/molxK	1007.98	Joback Method
cpg	1171.66	J/molxK	1041.25	Joback Method
cpg	1184.11	J/molxK	1074.52	Joback Method
dvisc	0.0007591	Paxs	489.40	Joback Method
dvisc	0.0003519	Paxs	553.65	Joback Method

dvisc	0.0001914	Paxs	617.90	Joback Method
dvisc	0.0001167	Paxs	682.14	Joback Method
dvisc	0.0000775	Paxs	746.39	Joback Method
dvisc	0.0000549	Paxs	810.64	Joback Method
dvisc	0.0000410	Paxs	874.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391549&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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