Glutaric acid, cyclohexylmethyl 3,7-dimethyloctyl ester

Inchi: InChI=1S/C22H40O4/c1-18(2)9-7-10-19(3)15-16-25-21(23)13-8-14-22(24)26-17-20-11-5

InchiKey: PYFZESWVFVUFFK-UHFFFAOYSA-N

Formula: C22H40O4

SMILES: CC(C)CCCC(C)CCOC(=O)CCCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-313.91	kJ/mol	Joback Method
hf	-943.25	kJ/mol	Joback Method
hfus	43.10	kJ/mol	Joback Method
hvap	82.53	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.676		Crippen Method
mcvol	324.860	ml/mol	McGowan Method
pc	1098.62	kPa	Joback Method
rinpol	2561.00		NIST Webbook
rinpol	2561.00		NIST Webbook
tb	874.01	K	Joback Method
tc	1075.68	K	Joback Method
tf	459.40	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1090.46	J/mol×K	874.01	Joback Method
cpg	1109.79	J/mol×K	907.62	Joback Method
cpg	1127.66	J/mol×K	941.23	Joback Method
cpg	1144.12	J/mol×K	974.85	Joback Method
cpg	1159.18	J/mol×K	1008.46	Joback Method
cpg	1172.88	J/mol×K	1042.07	Joback Method
cpg	1185.25	J/mol×K	1075.68	Joback Method
dvisc	0.0010552	Pa×s	459.40	Joback Method

dvisc	0.0004104	Pa×s	528.50	Joback Method
dvisc	0.0001985	Pa×s	597.60	Joback Method
dvisc	0.0001117	Pa×s	666.70	Joback Method
dvisc	0.0000700	Pa×s	735.81	Joback Method
dvisc	0.0000475	Pa×s	804.91	Joback Method
dvisc	0.0000343	Pa×s	874.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391486&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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