Glutaric acid, cyclohexylmethyl pentadecyl ester

Inchi: InChI=1S/C27H50O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-23-30-26(28)21-18-22-27(29)31
InchiKey: AFEHGFBULMZUQY-UHFFFAOYSA-N
Formula: C27H50O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 438.68

Physical Properties

Property code	Value	Unit	Source
gf	-266.93	kJ/mol	Joback Method
hf	-1035.89	kJ/mol	Joback Method
hfus	63.09	kJ/mol	Joback Method
hvap	94.44	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	7.915		Crippen Method
mcvol	395.310	ml/mol	McGowan Method
pc	810.30	kPa	Joback Method
rinpol	3208.00		NIST Webbook
rinpol	3208.00		NIST Webbook
tb	989.29	K	Joback Method
tc	1213.99	K	Joback Method
tf	545.75	K	Joback Method
vc	1.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1406.41	J/mol×K	989.29	Joback Method
cpg	1489.27	J/mol×K	1176.54	Joback Method
cpg	1476.25	J/mol×K	1139.09	Joback Method
cpg	1461.51	J/mol×K	1101.64	Joback Method
cpg	1445.00	J/mol×K	1064.19	Joback Method
cpg	1426.65	J/mol×K	1026.74	Joback Method
cpg	1500.65	J/mol×K	1213.99	Joback Method
dvisc	0.0000189	Pa×s	989.29	Joback Method

dvisc	0.0000256	Pa×s	915.37	Joback Method
dvisc	0.0000365	Pa×s	841.44	Joback Method
dvisc	0.0000559	Pa×s	767.52	Joback Method
dvisc	0.0000936	Pa×s	693.60	Joback Method
dvisc	0.0001774	Pa×s	619.67	Joback Method
dvisc	0.0003994	Pa×s	545.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391656&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