Glutaric acid, di(3,7-dimethyloctyl) ester

Inchi: InChI=1S/C25H48O4/c1-20(2)10-7-12-22(5)16-18-28-24(26)14-9-15-25(27)29-19-17-23(
InchiKey: NUXPEKJWRCBJBZ-UHFFFAOYSA-N
Formula: C25H48O4
SMILES: CC(C)CCCC(C)CCOC(=O)CCCC(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
gf	-317.98	kJ/mol	Joback Method
hf	-1070.05	kJ/mol	Joback Method
hfus	51.99	kJ/mol	Joback Method
hvap	88.00	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.948		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	819.13	kPa	Joback Method
rinpol	2656.00		NIST Webbook
rinpol	2656.00		NIST Webbook
tb	922.22	K	Joback Method
tc	1129.79	K	Joback Method
tf	455.83	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.74	J/mol×K	922.22	Joback Method
cpg	1303.07	J/mol×K	956.81	Joback Method
cpg	1321.86	J/mol×K	991.41	Joback Method
cpg	1339.16	J/mol×K	1026.00	Joback Method
cpg	1355.00	J/mol×K	1060.60	Joback Method
cpg	1369.43	J/mol×K	1095.19	Joback Method
cpg	1382.49	J/mol×K	1129.79	Joback Method
dvisc	0.0009015	Pa×s	455.83	Joback Method

dvisc	0.0002897	Pa×s	533.56	Joback Method
dvisc	0.0001242	Pa×s	611.29	Joback Method
dvisc	0.0000645	Pa×s	689.02	Joback Method
dvisc	0.0000382	Pa×s	766.76	Joback Method
dvisc	0.0000250	Pa×s	844.49	Joback Method
dvisc	0.0000175	Pa×s	922.22	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391496&Units=SI

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