Glutaric acid, 3-oxobut-2-yl tridecyl ester

Inchi: InChI=1S/C22H40O5/c1-4-5-6-7-8-9-10-11-12-13-14-18-26-21(24)16-15-17-22(25)27-20
InchiKey: MXEYIKMWSFGBCI-UHFFFAOYSA-N
Formula: C22H40O5
SMILES: CCCCCCCCCCCCCOC(=O)CCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 384.55

Physical Properties

Property code	Value	Unit	Source
gf	-464.84	kJ/mol	Joback Method
hf	-1104.87	kJ/mol	Joback Method
hfus	56.39	kJ/mol	Joback Method
hvap	89.24	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	5.532		Crippen Method
mcvol	337.290	ml/mol	McGowan Method
pc	997.02	kPa	Joback Method
rinpol	2687.00		NIST Webbook
tb	908.77	K	Joback Method
tc	1112.66	K	Joback Method
tf	516.95	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1114.67	J/mol×K	908.77	Joback Method
cpg	1132.27	J/mol×K	942.75	Joback Method
cpg	1148.54	J/mol×K	976.73	Joback Method
cpg	1163.50	J/mol×K	1010.72	Joback Method
cpg	1177.19	J/mol×K	1044.70	Joback Method
cpg	1189.62	J/mol×K	1078.68	Joback Method
cpg	1200.82	J/mol×K	1112.66	Joback Method
dvisc	0.0005844	Pa×s	516.95	Joback Method
dvisc	0.0002793	Pa×s	582.25	Joback Method

dvisc	0.0001549	Pa×s	647.56	Joback Method
dvisc	0.0000957	Pa×s	712.86	Joback Method
dvisc	0.0000641	Pa×s	778.16	Joback Method
dvisc	0.0000457	Pa×s	843.47	Joback Method
dvisc	0.0000342	Pa×s	908.77	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=U359713&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