Glutaric acid, oct-1-en-3-yl dodec-2-en-1-yl ester

Inchi: InChI=1S/C25H44O4/c1-4-7-9-10-11-12-13-14-15-17-22-28-24(26)20-18-21-25(27)29-23

InchiKey: HPQXRJVNRNVUPY-BMRADRMJSA-N

Formula: C25H44O4

SMILES: C=CC(CCCCC)OC(=O)CCCC(=O)OCC=CCCCCCCCCC

Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-142.60	kJ/mol	Joback Method
hf	-811.56	kJ/mol	Joback Method
hfus	61.48	kJ/mol	Joback Method
hvap	88.46	kJ/mol	Joback Method
log10ws	-7.83		Crippen Method
logp	7.075		Crippen Method
mcvol	369.390	ml/mol	McGowan Method
pc	852.97	kPa	Joback Method
rinpol	2713.00		NIST Webbook
rinpol	2713.00		NIST Webbook
tb	924.38	K	Joback Method
tc	1132.51	K	Joback Method
tf	493.99	K	Joback Method
vc	1.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1224.89	J/mol×K	924.38	Joback Method
cpg	1309.52	J/mol×K	1097.82	Joback Method
cpg	1295.00	J/mol×K	1063.13	Joback Method
cpg	1279.33	J/mol×K	1028.44	Joback Method
cpg	1262.46	J/mol×K	993.76	Joback Method
cpg	1244.33	J/mol×K	959.07	Joback Method
cpg	1322.96	J/mol×K	1132.51	Joback Method
dvisc	0.0000217	Pa×s	924.38	Joback Method

dvisc	0.0000295	Pa×s	852.65	Joback Method
dvisc	0.0000423	Pa×s	780.92	Joback Method
dvisc	0.0000652	Pa×s	709.18	Joback Method
dvisc	0.0001110	Pa×s	637.45	Joback Method
dvisc	0.0002161	Pa×s	565.72	Joback Method
dvisc	0.0005106	Pa×s	493.99	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=U405357&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