Glutaric acid, dodec-2-en-1-yl phenethyl ester

Inchi: InChI=1S/C25H38O4/c1-2-3-4-5-6-7-8-9-10-14-21-28-24(26)18-15-19-25(27)29-22-20-23
InchiKey: FZRHPKOBINQTFI-GXDHUFHOSA-N
Formula: C25H38O4
SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 402.57

Physical Properties

Property code	Value	Unit	Source
gf	-115.59	kJ/mol	Joback Method
hf	-695.18	kJ/mol	Joback Method
hfus	60.32	kJ/mol	Joback Method
hvap	91.79	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.183		Crippen Method
mcvol	349.930	ml/mol	McGowan Method
pc	1012.30	kPa	Joback Method
rinpol	2967.00		NIST Webbook
rinpol	2967.00		NIST Webbook
tb	954.82	K	Joback Method
tc	1169.21	K	Joback Method
tf	537.17	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1153.74	J/mol×K	954.82	Joback Method
cpg	1170.75	J/mol×K	990.55	Joback Method
cpg	1186.48	J/mol×K	1026.28	Joback Method
cpg	1200.99	J/mol×K	1062.02	Joback Method
cpg	1214.34	J/mol×K	1097.75	Joback Method
cpg	1226.59	J/mol×K	1133.48	Joback Method
cpg	1237.81	J/mol×K	1169.21	Joback Method
dvisc	0.0003657	Pa×s	537.17	Joback Method

dvisc	0.0001765	Pa×s	606.78	Joback Method
dvisc	0.0000990	Pa×s	676.39	Joback Method
dvisc	0.0000618	Pa×s	745.99	Joback Method
dvisc	0.0000419	Pa×s	815.60	Joback Method
dvisc	0.0000301	Pa×s	885.21	Joback Method
dvisc	0.0000227	Pa×s	954.82	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=U391799&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