Glutaric acid, dodec-2-en-1-yl 4-acetylphenyl ester

Inchi: InChI=1S/C25H36O5/c1-3-4-5-6-7-8-9-10-11-12-20-29-24(27)14-13-15-25(28)30-23-18-1

InchiKey: ODTDYRWQEMVAQN-VAWYXSNFSA-N

Formula: C25H36O5

SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)Oc1ccc(C(C)=O)cc1

Mol. weight [g/mol]: 416.55

Physical Properties

Property code	Value	Unit	Source
gf	-254.14	kJ/mol	Joback Method
hf	-819.23	kJ/mol	Joback Method
hfus	61.53	kJ/mol	Joback Method
hvap	99.20	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	6.205		Crippen Method
mcvol	351.500	ml/mol	McGowan Method
pc	1043.95	kPa	Joback Method
rinpol	3223.00		NIST Webbook
rinpol	3223.00		NIST Webbook
tb	1013.67	K	Joback Method
tc	1241.10	K	Joback Method
tf	599.62	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1166.80	J/mol×K	1013.67	Joback Method
cpg	1181.88	J/mol×K	1051.57	Joback Method
cpg	1195.58	J/mol×K	1089.48	Joback Method
cpg	1207.95	J/mol×K	1127.38	Joback Method
cpg	1219.06	J/mol×K	1165.29	Joback Method
cpg	1228.98	J/mol×K	1203.19	Joback Method
cpg	1237.77	J/mol×K	1241.10	Joback Method
dvisc	0.0002554	Pa×s	599.62	Joback Method

dvisc	0.0001373	Pa×s	668.63	Joback Method
dvisc	0.0000829	Pa×s	737.64	Joback Method
dvisc	0.0000546	Pa×s	806.64	Joback Method
dvisc	0.0000384	Pa×s	875.65	Joback Method
dvisc	0.0000284	Pa×s	944.66	Joback Method
dvisc	0.0000219	Pa×s	1013.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392039&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

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