Glutaric acid, dodec-2-en-1-yl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C25H38O5/c1-4-5-6-7-8-9-10-11-12-13-19-29-24(26)15-14-16-25(27)30-23-20

InchiKey: MWXJDLJMTODJMX-OUKQBFOZSA-N

Formula: C25H38O5

SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)Oc1cc(C)ccc1OC

Mol. weight [g/mol]: 418.57

Physical Properties

Property code	Value	Unit	Source
gf	-239.85	kJ/mol	Joback Method
hf	-850.34	kJ/mol	Joback Method
hfus	60.73	kJ/mol	Joback Method
hvap	95.52	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	6.319		Crippen Method
mcvol	355.800	ml/mol	McGowan Method
pc	982.69	kPa	Joback Method
rinpol	3047.00		NIST Webbook
rinpol	3047.00		NIST Webbook
tb	987.20	K	Joback Method
tc	1208.67	K	Joback Method
tf	584.44	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.69	J/mol×K	987.20	Joback Method
cpg	1197.80	J/mol×K	1024.11	Joback Method
cpg	1212.39	J/mol×K	1061.02	Joback Method
cpg	1225.50	J/mol×K	1097.93	Joback Method
cpg	1237.17	J/mol×K	1134.85	Joback Method
cpg	1247.43	J/mol×K	1171.76	Joback Method
cpg	1256.34	J/mol×K	1208.67	Joback Method
dvisc	0.0001930	Pa×s	584.44	Joback Method

dvisc	0.0001054	Pa×s	651.57	Joback Method
dvisc	0.0000645	Pa×s	718.69	Joback Method
dvisc	0.0000429	Pa×s	785.82	Joback Method
dvisc	0.0000304	Pa×s	852.95	Joback Method
dvisc	0.0000227	Pa×s	920.07	Joback Method
dvisc	0.0000176	Pa×s	987.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393933&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

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