Glutaric acid, dec-2-yl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C23H36O5/c1-5-6-7-8-9-10-12-19(3)27-22(24)13-11-14-23(25)28-21-17-18(2)1

InchiKey: MRGXYTCQVIUYAJ-UHFFFAOYSA-N

Formula: C23H36O5

SMILES: CCCCCCCCC(C)OC(=O)CCCC(=O)Oc1cc(C)ccc1OC

Mol. weight [g/mol]: 392.53

Physical Properties

Property code	Value	Unit	Source
gf	-339.35	kJ/mol	Joback Method
hf	-931.56	kJ/mol	Joback Method
hfus	51.83	kJ/mol	Joback Method
hvap	90.73	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.762		Crippen Method
mcvol	331.920	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	2734.00		NIST Webbook
rinpol	2734.00		NIST Webbook
tb	936.84	K	Joback Method
tc	1147.96	K	Joback Method
tf	551.98	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.61	J/mol×K	936.84	Joback Method
cpg	1103.67	J/mol×K	972.03	Joback Method
cpg	1118.26	J/mol×K	1007.21	Joback Method
cpg	1131.39	J/mol×K	1042.40	Joback Method
cpg	1143.07	J/mol×K	1077.59	Joback Method
cpg	1153.31	J/mol×K	1112.78	Joback Method
cpg	1162.14	J/mol×K	1147.96	Joback Method
dvisc	0.0002883	Pa×s	551.98	Joback Method

dvisc	0.0001546	Pa×s	616.12	Joback Method
dvisc	0.0000933	Pa×s	680.27	Joback Method
dvisc	0.0000614	Pa×s	744.41	Joback Method
dvisc	0.0000432	Pa×s	808.55	Joback Method
dvisc	0.0000320	Pa×s	872.70	Joback Method
dvisc	0.0000247	Pa×s	936.84	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=U393931&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