Glutaric acid, 3-methylbut-2-en-1-yl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C18H24O5/c1-13(2)10-11-22-17(19)6-5-7-18(20)23-16-12-14(3)8-9-15(16)21-4

InchiKey: FQNHBYPALNGZPL-UHFFFAOYSA-N

Formula: C18H24O5

SMILES: COc1ccc(C)cc1OC(=O)CCCC(=O)OCC=C(C)C

Mol. weight [g/mol]: 320.38

Physical Properties

Property code	Value	Unit	Source
gf	-307.34	kJ/mol	Joback Method
hf	-715.65	kJ/mol	Joback Method
hfus	41.29	kJ/mol	Joback Method
hvap	80.02	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.589		Crippen Method
mcvol	257.170	ml/mol	McGowan Method
pc	1583.49	kPa	Joback Method
rinpol	2355.00		NIST Webbook
rinpol	2355.00		NIST Webbook
tb	826.92	K	Joback Method
tc	1034.45	K	Joback Method
tf	491.59	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.66	J/mol×K	826.92	Joback Method
cpg	777.46	J/mol×K	861.51	Joback Method
cpg	791.19	J/mol×K	896.10	Joback Method
cpg	803.84	J/mol×K	930.68	Joback Method
cpg	815.45	J/mol×K	965.27	Joback Method
cpg	826.00	J/mol×K	999.86	Joback Method
cpg	835.53	J/mol×K	1034.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393923&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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