Glutaric acid, 3-methylbut-2-en-1-yl 2-methoxyphenyl ester

Inchi: InChI=1S/C17H22O5/c1-13(2)11-12-21-16(18)9-6-10-17(19)22-15-8-5-4-7-14(15)20-3/h4

InchiKey: XXLAEWQJZUKYIX-UHFFFAOYSA-N

Formula: C17H22O5

SMILES: COc1ccccc1OC(=O)CCCC(=O)OCC=C(C)C

Mol. weight [g/mol]: 306.35

Physical Properties

Property code	Value	Unit	Source
gf	-306.13	kJ/mol	Joback Method
hf	-683.54	kJ/mol	Joback Method
hfus	39.09	kJ/mol	Joback Method
hvap	77.13	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.280		Crippen Method
mcvol	243.080	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tb	799.06	K	Joback Method
tc	1006.83	K	Joback Method
tf	467.80	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.73	J/mol×K	799.06	Joback Method
cpg	721.38	J/mol×K	833.69	Joback Method
cpg	735.00	J/mol×K	868.32	Joback Method
cpg	747.58	J/mol×K	902.94	Joback Method
cpg	759.15	J/mol×K	937.57	Joback Method
cpg	769.72	J/mol×K	972.20	Joback Method
cpg	779.31	J/mol×K	1006.83	Joback Method

Sources

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=U391756&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:
https://www.chemeo.com/cid/93-141-2/Glutaric-acid-3-methylbut-2-en-1-yl-2-methoxyphenyl-ester.pdf
Generated by Cheméo on 2024-05-06 05:29:47.261843104 +0000 UTC m=+17262636.182420417.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.