Glutaric acid, 3-methylbut-2-en-1-yl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C17H21BrO5/c1-12(2)9-10-22-16(19)5-4-6-17(20)23-14-8-7-13(18)11-15(14)21

InchiKey: BTYZZBCXLBNKHY-UHFFFAOYSA-N

Formula: C17H21BrO5

SMILES: COc1cc(Br)ccc1OC(=O)CCCC(=O)OCC=C(C)C

Mol. weight [g/mol]: 385.25

Physical Properties

Property code	Value	Unit	Source
gf	-301.44	kJ/mol	Joback Method
hf	-668.68	kJ/mol	Joback Method
hfus	43.99	kJ/mol	Joback Method
hvap	84.23	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.043		Crippen Method
mcvol	260.580	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2551.00		NIST Webbook
rinpol	2551.00		NIST Webbook
tb	870.20	K	Joback Method
tc	1088.88	K	Joback Method
tf	540.12	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.42	J/mol×K	870.20	Joback Method
cpg	755.32	J/mol×K	906.65	Joback Method
cpg	767.14	J/mol×K	943.09	Joback Method
cpg	777.92	J/mol×K	979.54	Joback Method
cpg	787.68	J/mol×K	1015.99	Joback Method
cpg	796.42	J/mol×K	1052.43	Joback Method
cpg	804.18	J/mol×K	1088.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393884&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