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

Inchi: InChI=1S/C17H23BrO5/c1-11(2)12(3)22-16(19)6-5-7-17(20)23-14-9-8-13(18)10-15(14)21

InchiKey: HGUCGTFGSMQFSA-UHFFFAOYSA-N

Formula: C17H23BrO5

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

Mol. weight [g/mol]: 387.27

Physical Properties

Property code	Value	Unit	Source
gf	-377.99	kJ/mol	Joback Method
hf	-786.67	kJ/mol	Joback Method
hfus	38.05	kJ/mol	Joback Method
hvap	83.42	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.121		Crippen Method
mcvol	264.880	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	2436.00		NIST Webbook
rinpol	2436.00		NIST Webbook
tb	865.28	K	Joback Method
tc	1081.52	K	Joback Method
tf	529.16	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.27	J/mol×K	865.28	Joback Method
cpg	784.71	J/mol×K	901.32	Joback Method
cpg	796.97	J/mol×K	937.36	Joback Method
cpg	808.04	J/mol×K	973.40	Joback Method
cpg	817.93	J/mol×K	1009.44	Joback Method
cpg	826.64	J/mol×K	1045.48	Joback Method
cpg	834.18	J/mol×K	1081.52	Joback Method
dvisc	0.0004004	Pa×s	529.16	Joback Method

dvisc	0.0002301	Pa×s	585.18	Joback Method
dvisc	0.0001457	Pa×s	641.20	Joback Method
dvisc	0.0000993	Pa×s	697.22	Joback Method
dvisc	0.0000716	Pa×s	753.24	Joback Method
dvisc	0.0000541	Pa×s	809.26	Joback Method
dvisc	0.0000423	Pa×s	865.28	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=U393703&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