Glutaric acid, 2-methylpent-3-yl 4-bromophenyl ester

Inchi: InChI=1S/C17H23BrO4/c1-4-15(12(2)3)22-17(20)7-5-6-16(19)21-14-10-8-13(18)9-11-14/

InchiKey: XDZYYGIMZWXSTG-UHFFFAOYSA-N

Formula: C17H23BrO4

SMILES: CCC(OC(=O)CCCC(=O)Oc1ccc(Br)cc1)C(C)C

Mol. weight [g/mol]: 371.27

Physical Properties

Property code	Value	Unit	Source
gf	-263.36	kJ/mol	Joback Method
hf	-642.98	kJ/mol	Joback Method
hfus	37.25	kJ/mol	Joback Method
hvap	80.34	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.503		Crippen Method
mcvol	259.010	ml/mol	McGowan Method
pc	1800.03	kPa	Joback Method
rinpol	2367.00		NIST Webbook
rinpol	2367.00		NIST Webbook
tb	837.88	K	Joback Method
tc	1053.87	K	Joback Method
tf	494.41	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.13	J/mol×K	837.88	Joback Method
cpg	759.22	J/mol×K	873.88	Joback Method
cpg	772.20	J/mol×K	909.88	Joback Method
cpg	784.09	J/mol×K	945.88	Joback Method
cpg	794.93	J/mol×K	981.87	Joback Method
cpg	804.74	J/mol×K	1017.87	Joback Method
cpg	813.54	J/mol×K	1053.87	Joback Method
dvisc	0.0006689	Pa×s	494.41	Joback Method

dvisc	0.0003571	Pa×s	551.65	Joback Method
dvisc	0.0002145	Pa×s	608.90	Joback Method
dvisc	0.0001407	Pa×s	666.14	Joback Method
dvisc	0.0000986	Pa×s	723.39	Joback Method
dvisc	0.0000728	Pa×s	780.63	Joback Method
dvisc	0.0000561	Pa×s	837.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393287&Units=SI

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