Glutaric acid, 4-bromo-2-methoxyphenyl ethyl ester

Inchi: InChI=1S/C14H17BrO5/c1-3-19-13(16)5-4-6-14(17)20-11-8-7-10(15)9-12(11)18-2/h7-9H

InchiKey: KXLUJJPWVGOXEI-UHFFFAOYSA-N

Formula: C14H17BrO5

SMILES: CCOC(=O)CCCC(=O)Oc1ccc(Br)cc1OC

Mol. weight [g/mol]: 345.19

Physical Properties

Property code	Value	Unit	Source
gf	-398.37	kJ/mol	Joback Method
hf	-714.19	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	77.52	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.096		Crippen Method
mcvol	222.610	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	2221.00		NIST Webbook
rinpol	2221.00		NIST Webbook
tb	797.52	K	Joback Method
tc	1012.86	K	Joback Method
tf	525.35	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.37	J/mol×K	797.52	Joback Method
cpg	614.80	J/mol×K	833.41	Joback Method
cpg	626.24	J/mol×K	869.30	Joback Method
cpg	636.71	J/mol×K	905.19	Joback Method
cpg	646.19	J/mol×K	941.08	Joback Method
cpg	654.68	J/mol×K	976.97	Joback Method
cpg	662.17	J/mol×K	1012.86	Joback Method
dvisc	0.0004471	Pa×s	525.35	Joback Method

dvisc	0.0002970	Pa×s	570.71	Joback Method
dvisc	0.0002096	Pa×s	616.07	Joback Method
dvisc	0.0001551	Pa×s	661.43	Joback Method
dvisc	0.0001193	Pa×s	706.80	Joback Method
dvisc	0.0000948	Pa×s	752.16	Joback Method
dvisc	0.0000772	Pa×s	797.52	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=U393898&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
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