Glutaric acid, 2-(2-bromophenyl)ethyl butyl ester

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

InchiKey: UAHNHSSHJPIQMY-UHFFFAOYSA-N

Formula: C17H23BrO4

SMILES: CCCCOC(=O)CCCC(=O)OCCc1ccccc1Br

Mol. weight [g/mol]: 371.27

Physical Properties

Property code	Value	Unit	Source
gf	-258.48	kJ/mol	Joback Method
hf	-632.42	kJ/mol	Joback Method
hfus	44.30	kJ/mol	Joback Method
hvap	81.12	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.048		Crippen Method
mcvol	259.010	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	2510.00		NIST Webbook
rinpol	2510.00		NIST Webbook
tb	838.76	K	Joback Method
tc	1049.57	K	Joback Method
tf	524.41	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.01	J/mol×K	838.76	Joback Method
cpg	757.80	J/mol×K	873.90	Joback Method
cpg	770.55	J/mol×K	909.03	Joback Method
cpg	782.28	J/mol×K	944.17	Joback Method
cpg	793.04	J/mol×K	979.30	Joback Method
cpg	802.83	J/mol×K	1014.44	Joback Method
cpg	811.68	J/mol×K	1049.57	Joback Method
dvisc	0.0005356	Pa×s	524.41	Joback Method

dvisc	0.0003233	Pa×s	576.80	Joback Method
dvisc	0.0002123	Pa×s	629.19	Joback Method
dvisc	0.0001487	Pa×s	681.59	Joback Method
dvisc	0.0001096	Pa×s	733.98	Joback Method
dvisc	0.0000841	Pa×s	786.37	Joback Method
dvisc	0.0000667	Pa×s	838.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377399&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

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