

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

Inchi:	InChI=1S/C17H23BrO4/c1-13(2)12-22-17(20)9-5-8-16(19)21-11-10-14-6-3-4-7-15(14)18
InchiKey:	JOPLMVFDEDWCOW-UHFFFAOYSA-N
Formula:	C17H23BrO4
SMILES:	CC(C)COC(=O)CCCC(=O)OCCc1ccccc1Br
Mol. weight [g/mol]:	371.27

Physical Properties

Property code	Value	Unit	Source
gf	-260.92	kJ/mol	Joback Method
hf	-637.70	kJ/mol	Joback Method
hfus	40.77	kJ/mol	Joback Method
hvap	80.73	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	3.904		Crippen Method
mcvol	259.010	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpola	2465.00		NIST Webbook
rinpola	2465.00		NIST Webbook
tb	838.32	K	Joback Method
tc	1051.65	K	Joback Method
tf	509.41	K	Joback Method
vc	0.984	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.57	J/molxK	838.32	Joback Method
cpg	758.50	J/molxK	873.87	Joback Method
cpg	771.36	J/molxK	909.43	Joback Method
cpg	783.18	J/molxK	944.98	Joback Method
cpg	793.97	J/molxK	980.54	Joback Method
cpg	803.77	J/molxK	1016.09	Joback Method
cpg	812.60	J/molxK	1051.65	Joback Method
dvisc	0.0005943	Paxs	509.41	Joback Method

dvisc	0.0003384	Paxs	564.23	Joback Method
dvisc	0.0002129	Paxs	619.05	Joback Method
dvisc	0.0001444	Paxs	673.87	Joback Method
dvisc	0.0001039	Paxs	728.68	Joback Method
dvisc	0.0000782	Paxs	783.50	Joback Method
dvisc	0.0000612	Paxs	838.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377398&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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