Glutaric acid, 8-chlorooctyl 4-bromophenyl ester

Inchi: InChI=1S/C19H26BrClO4/c20-16-10-12-17(13-11-16)25-19(23)9-7-8-18(22)24-15-6-4-2-1

InchiKey: QKSIFXNXKPPKKN-UHFFFAOYSA-N

Formula: C19H26BrClO4

SMILES: O=C(CCCC(=O)Oc1ccc(Br)cc1)OCCCCCCCCCl

Mol. weight [g/mol]: 433.76

Physical Properties

Property code	Value	Unit	Source
gf	-253.57	kJ/mol	Joback Method
hf	-689.44	kJ/mol	Joback Method
hfus	53.67	kJ/mol	Joback Method
hvap	89.96	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	5.647		Crippen Method
mcvol	299.430	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	3070.00		NIST Webbook
rinpol	3070.00		NIST Webbook
tb	921.95	K	Joback Method
tc	1137.59	K	Joback Method
tf	576.87	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.36	J/mol×K	921.95	Joback Method
cpg	938.06	J/mol×K	1101.65	Joback Method
cpg	929.19	J/mol×K	1065.71	Joback Method
cpg	919.33	J/mol×K	1029.77	Joback Method
cpg	908.42	J/mol×K	993.83	Joback Method
cpg	896.45	J/mol×K	957.89	Joback Method
cpg	945.95	J/mol×K	1137.59	Joback Method
dvisc	0.0000421	Pa×s	921.95	Joback Method

dvisc	0.0000533	Pa×s	864.44	Joback Method
dvisc	0.0000699	Pa×s	806.92	Joback Method
dvisc	0.0000954	Pa×s	749.41	Joback Method
dvisc	0.0001372	Pa×s	691.90	Joback Method
dvisc	0.0002107	Pa×s	634.38	Joback Method
dvisc	0.0003525	Pa×s	576.87	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=U393298&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