Glutaric acid, di(4-bromophenyl) ester

Inchi: InChI=1S/C17H14Br2O4/c18-12-4-8-14(9-5-12)22-16(20)2-1-3-17(21)23-15-10-6-13(19)
InchiKey: LICBOYUGEOPRET-UHFFFAOYSA-N
Formula: C17H14Br2O4
SMILES: O=C(CCCC(=O)Oc1ccc(Br)cc1)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 442.10

Physical Properties

Property code	Value	Unit	Source
gf	-141.38	kJ/mol	Joback Method
hf	-381.03	kJ/mol	Joback Method
hfus	43.23	kJ/mol	Joback Method
hvap	90.49	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	4.893		Crippen Method
mcvol	252.750	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	3059.00		NIST Webbook
rinpol	3059.00		NIST Webbook
tb	936.58	K	Joback Method
tc	1187.07	K	Joback Method
tf	623.15	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.87	J/mol×K	936.58	Joback Method
cpg	710.57	J/mol×K	1145.32	Joback Method
cpg	704.85	J/mol×K	1103.57	Joback Method
cpg	698.18	J/mol×K	1061.83	Joback Method
cpg	690.49	J/mol×K	1020.08	Joback Method
cpg	681.74	J/mol×K	978.33	Joback Method
cpg	715.40	J/mol×K	1187.07	Joback Method
dvisc	0.0000540	Pa×s	936.58	Joback Method

dvisc	0.0000660	Pa×s	884.34	Joback Method
dvisc	0.0000827	Pa×s	832.10	Joback Method
dvisc	0.0001069	Pa×s	779.87	Joback Method
dvisc	0.0001433	Pa×s	727.63	Joback Method
dvisc	0.0002009	Pa×s	675.39	Joback Method
dvisc	0.0002982	Pa×s	623.15	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=U358734&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