Glutaric acid, di(3-bromobenzyl) ester

Inchi: InChI=1S/C19H18Br2O4/c20-16-6-1-4-14(10-16)12-24-18(22)8-3-9-19(23)25-13-15-5-2-
InchiKey: UTHIYRFZEOVVEE-UHFFFAOYSA-N
Formula: C19H18Br2O4
SMILES: O=C(CCCC(=O)OCc1cccc(Br)c1)OCc1cccc(Br)c1
Mol. weight [g/mol]: 470.15

Physical Properties

Property code	Value	Unit	Source
gf	-124.54	kJ/mol	Joback Method
hf	-422.31	kJ/mol	Joback Method
hfus	48.41	kJ/mol	Joback Method
hvap	94.95	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.169		Crippen Method
mcvol	280.930	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	3420.00		NIST Webbook
rinpol	3420.00		NIST Webbook
tb	982.34	K	Joback Method
tc	1227.67	K	Joback Method
tf	645.69	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.03	J/mol×K	982.34	Joback Method
cpg	825.58	J/mol×K	1186.78	Joback Method
cpg	819.49	J/mol×K	1145.89	Joback Method
cpg	812.46	J/mol×K	1105.01	Joback Method
cpg	804.41	J/mol×K	1064.12	Joback Method
cpg	795.29	J/mol×K	1023.23	Joback Method
cpg	830.79	J/mol×K	1227.67	Joback Method
dvisc	0.0000399	Pa×s	982.34	Joback Method

dvisc	0.0000491	Pa×s	926.23	Joback Method
dvisc	0.0000621	Pa×s	870.12	Joback Method
dvisc	0.0000811	Pa×s	814.02	Joback Method
dvisc	0.0001102	Pa×s	757.91	Joback Method
dvisc	0.0001572	Pa×s	701.80	Joback Method
dvisc	0.0002386	Pa×s	645.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377753&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