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

Inchi: InChI=1S/C21H22Br2O4/c22-18-8-3-1-6-16(18)12-14-26-20(24)10-5-11-21(25)27-15-13-
InchiKey: GXMIVDIVCAWBES-UHFFFAOYSA-N
Formula: C21H22Br2O4
SMILES: O=C(CCCC(=O)OCCc1ccccc1Br)OCCc1ccccc1Br
Mol. weight [g/mol]: 498.20

Physical Properties

Property code	Value	Unit	Source
gf	-107.70	kJ/mol	Joback Method
hf	-463.59	kJ/mol	Joback Method
hfus	53.59	kJ/mol	Joback Method
hvap	99.40	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.253		Crippen Method
mcvol	309.110	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	3401.00		NIST Webbook
rinpol	3401.00		NIST Webbook
tb	1028.10	K	Joback Method
tc	1271.63	K	Joback Method
tf	668.23	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.82	J/mol×K	1028.10	Joback Method
cpg	942.78	J/mol×K	1231.04	Joback Method
cpg	936.41	J/mol×K	1190.45	Joback Method
cpg	929.11	J/mol×K	1149.87	Joback Method
cpg	920.79	J/mol×K	1109.28	Joback Method
cpg	911.38	J/mol×K	1068.69	Joback Method
cpg	948.27	J/mol×K	1271.63	Joback Method
dvisc	0.0000293	Pa×s	1028.10	Joback Method

dvisc	0.0000363	Pa×s	968.12	Joback Method
dvisc	0.0000462	Pa×s	908.14	Joback Method
dvisc	0.0000610	Pa×s	848.16	Joback Method
dvisc	0.0000839	Pa×s	788.19	Joback Method
dvisc	0.0001217	Pa×s	728.21	Joback Method
dvisc	0.0001887	Pa×s	668.23	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=U377406&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

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