Glutaric acid, 2-bromobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C19H27BrO4/c1-4-8-17(14(2)3)24-19(22)12-7-11-18(21)23-13-15-9-5-6-10-16(

InchiKey: GXQZLNLMMRITSC-UHFFFAOYSA-N

Formula: C19H27BrO4

SMILES: CCCC(OC(=O)CCCC(=O)OCc1ccccc1Br)C(C)C

Mol. weight [g/mol]: 399.32

Physical Properties

Property code	Value	Unit	Source
gf	-246.52	kJ/mol	Joback Method
hf	-684.26	kJ/mol	Joback Method
hfus	42.43	kJ/mol	Joback Method
hvap	84.80	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.030		Crippen Method
mcvol	287.190	ml/mol	McGowan Method
pc	1539.08	kPa	Joback Method
rinpol	2511.00		NIST Webbook
rinpol	2511.00		NIST Webbook
tb	883.64	K	Joback Method
tc	1098.00	K	Joback Method
tf	516.95	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.39	J/mol×K	883.64	Joback Method
cpg	874.83	J/mol×K	919.37	Joback Method
cpg	888.10	J/mol×K	955.09	Joback Method
cpg	900.24	J/mol×K	990.82	Joback Method
cpg	911.27	J/mol×K	1026.55	Joback Method
cpg	921.22	J/mol×K	1062.27	Joback Method
cpg	930.14	J/mol×K	1098.00	Joback Method
dvisc	0.0005344	Pa×s	516.95	Joback Method

dvisc	0.0002789	Pa×s	578.07	Joback Method
dvisc	0.0001649	Pa×s	639.18	Joback Method
dvisc	0.0001068	Pa×s	700.30	Joback Method
dvisc	0.0000742	Pa×s	761.41	Joback Method
dvisc	0.0000544	Pa×s	822.52	Joback Method
dvisc	0.0000417	Pa×s	883.64	Joback Method

Sources

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=U376763&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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