Glutaric acid, 2-(3-bromophenyl)ethyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C20H29BrO4/c1-4-7-18(15(2)3)25-20(23)11-6-10-19(22)24-13-12-16-8-5-9-17(

InchiKey: VGYVRGQVRCFKDX-UHFFFAOYSA-N

Formula: C20H29BrO4

SMILES: CCCC(OC(=O)CCCC(=O)OCCc1cccc(Br)c1)C(C)C

Mol. weight [g/mol]: 413.35

Physical Properties

Property code	Value	Unit	Source
gf	-238.10	kJ/mol	Joback Method
hf	-704.90	kJ/mol	Joback Method
hfus	45.02	kJ/mol	Joback Method
hvap	87.02	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.073		Crippen Method
mcvol	301.280	ml/mol	McGowan Method
pc	1429.38	kPa	Joback Method
rinpol	2660.00		NIST Webbook
rinpol	2660.00		NIST Webbook
tb	906.52	K	Joback Method
tc	1121.15	K	Joback Method
tf	528.22	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.14	J/mol×K	906.52	Joback Method
cpg	933.74	J/mol×K	942.29	Joback Method
cpg	947.14	J/mol×K	978.06	Joback Method
cpg	959.36	J/mol×K	1013.84	Joback Method
cpg	970.45	J/mol×K	1049.61	Joback Method
cpg	980.44	J/mol×K	1085.38	Joback Method
cpg	989.37	J/mol×K	1121.15	Joback Method
dvisc	0.0004752	Pa×s	528.22	Joback Method

dvisc	0.0002454	Pa×s	591.27	Joback Method
dvisc	0.0001440	Pa×s	654.32	Joback Method
dvisc	0.0000928	Pa×s	717.37	Joback Method
dvisc	0.0000642	Pa×s	780.42	Joback Method
dvisc	0.0000469	Pa×s	843.47	Joback Method
dvisc	0.0000358	Pa×s	906.52	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=U377208&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