Glutaric acid, 8-bromooctyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C20H37BrO4/c1-4-12-18(17(2)3)25-20(23)14-11-13-19(22)24-16-10-8-6-5-7-9-

InchiKey: JKABGAHLUMCFLL-UHFFFAOYSA-N

Formula: C20H37BrO4

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

Mol. weight [g/mol]: 421.41

Physical Properties

Property code	Value	Unit	Source
gf	-340.88	kJ/mol	Joback Method
hf	-929.96	kJ/mol	Joback Method
hfus	51.37	kJ/mol	Joback Method
hvap	84.08	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.803		Crippen Method
mcvol	325.040	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
rinpol	2663.00		NIST Webbook
rinpol	2663.00		NIST Webbook
tb	874.86	K	Joback Method
tc	1073.05	K	Joback Method
tf	489.28	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1018.04	J/mol×K	874.86	Joback Method
cpg	1034.99	J/mol×K	907.89	Joback Method
cpg	1050.81	J/mol×K	940.92	Joback Method
cpg	1065.51	J/mol×K	973.96	Joback Method
cpg	1079.12	J/mol×K	1006.99	Joback Method
cpg	1091.69	J/mol×K	1040.02	Joback Method
cpg	1103.23	J/mol×K	1073.05	Joback Method
dvisc	0.0006668	Pa×s	489.28	Joback Method

dvisc	0.0003054	Pa×s	553.54	Joback Method
dvisc	0.0001646	Pa×s	617.81	Joback Method
dvisc	0.0000996	Pa×s	682.07	Joback Method
dvisc	0.0000658	Pa×s	746.33	Joback Method
dvisc	0.0000464	Pa×s	810.60	Joback Method
dvisc	0.0000344	Pa×s	874.86	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=U377243&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