Glutaric acid, 8-bromooctyl 8-chlorooctyl ester

Inchi: InChI=1S/C21H38BrClO4/c22-16-9-5-1-3-7-11-18-26-20(24)14-13-15-21(25)27-19-12-8-4
InchiKey: KOHHGYXNDYOYJG-UHFFFAOYSA-N
Formula: C21H38BrClO4
SMILES: O=C(CCCC(=O)OCCCCCCCCCBr)OCCCCCCCCCCl
Mol. weight [g/mol]: 469.88

Physical Properties

Property code	Value	Unit	Source
gf	-339.51	kJ/mol	Joback Method
hf	-955.78	kJ/mol	Joback Method
hfus	65.20	kJ/mol	Joback Method
hvap	91.47	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	6.558		Crippen Method
mcvol	351.370	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
rinpol	3245.00		NIST Webbook
rinpol	3245.00		NIST Webbook
tb	936.05	K	Joback Method
tc	1146.13	K	Joback Method
tf	560.47	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1106.11	J/mol×K	936.05	Joback Method
cpg	1176.16	J/mol×K	1111.12	Joback Method
cpg	1164.45	J/mol×K	1076.10	Joback Method
cpg	1151.63	J/mol×K	1041.09	Joback Method
cpg	1137.66	J/mol×K	1006.08	Joback Method
cpg	1122.50	J/mol×K	971.06	Joback Method
cpg	1186.80	J/mol×K	1146.13	Joback Method
dvisc	0.0000293	Pa×s	936.05	Joback Method

dvisc	0.0000383	Pa×s	873.45	Joback Method
dvisc	0.0000521	Pa×s	810.86	Joback Method
dvisc	0.0000746	Pa×s	748.26	Joback Method
dvisc	0.0001141	Pa×s	685.66	Joback Method
dvisc	0.0001900	Pa×s	623.07	Joback Method
dvisc	0.0003546	Pa×s	560.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377245&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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