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

Inchi: InChI=1S/C22H33BrO4/c1-2-3-4-5-6-7-10-17-26-21(24)14-11-15-22(25)27-18-16-19-12-8

InchiKey: POBXMMSTLVWTMM-UHFFFAOYSA-N

Formula: C22H33BrO4

SMILES: CCCCCCCCCOC(=O)CCCC(=O)OCCc1ccccc1Br

Mol. weight [g/mol]: 441.40

Physical Properties

Property code	Value	Unit	Source
gf	-216.38	kJ/mol	Joback Method
hf	-735.62	kJ/mol	Joback Method
hfus	57.25	kJ/mol	Joback Method
hvap	92.25	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.999		Crippen Method
mcvol	329.460	ml/mol	McGowan Method
pc	1228.56	kPa	Joback Method
rinpol	3033.00		NIST Webbook
tb	953.16	K	Joback Method
tc	1169.05	K	Joback Method
tf	580.76	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.74	J/mol×K	953.16	Joback Method
cpg	1052.63	J/mol×K	989.14	Joback Method
cpg	1066.27	J/mol×K	1025.12	Joback Method
cpg	1078.70	J/mol×K	1061.10	Joback Method
cpg	1089.98	J/mol×K	1097.08	Joback Method
cpg	1100.14	J/mol×K	1133.06	Joback Method
cpg	1109.23	J/mol×K	1169.05	Joback Method
dvisc	0.0003088	Pa×s	580.76	Joback Method
dvisc	0.0001759	Pa×s	642.83	Joback Method

dvisc	0.0001106	Pa×s	704.89	Joback Method
dvisc	0.0000750	Pa×s	766.96	Joback Method
dvisc	0.0000539	Pa×s	829.03	Joback Method
dvisc	0.0000406	Pa×s	891.09	Joback Method
dvisc	0.0000317	Pa×s	953.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377404&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

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