Glutaric acid, 2-bromobenzyl heptadecyl ester

Inchi: InChI=1S/C29H47BrO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-24-33-28(31)22-19-23-
InchiKey: MVVOMXHSZMBANZ-UHFFFAOYSA-N
Formula: C29H47BrO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccccc1Br
Mol. weight [g/mol]: 539.59

Physical Properties

Property code	Value	Unit	Source
gf	-157.44	kJ/mol	Joback Method
hf	-880.10	kJ/mol	Joback Method
hfus	75.38	kJ/mol	Joback Method
hvap	107.83	kJ/mol	Joback Method
log10ws	-10.45		Crippen Method
logp	9.077		Crippen Method
mcvol	428.090	ml/mol	McGowan Method
pc	804.79	kPa	Joback Method
rinpol	3721.00		NIST Webbook
rinpol	3721.00		NIST Webbook
tb	1113.32	K	Joback Method
tc	1377.89	K	Joback Method
tf	659.65	K	Joback Method
vc	1.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1471.65	J/mol×K	1113.32	Joback Method
cpg	1488.76	J/mol×K	1157.41	Joback Method
cpg	1503.95	J/mol×K	1201.51	Joback Method
cpg	1517.35	J/mol×K	1245.60	Joback Method
cpg	1529.07	J/mol×K	1289.70	Joback Method
cpg	1539.25	J/mol×K	1333.79	Joback Method
cpg	1548.01	J/mol×K	1377.89	Joback Method
dvisc	0.0001268	Pa×s	659.65	Joback Method

dvisc	0.0000675	Pa×s	735.26	Joback Method
dvisc	0.0000404	Pa×s	810.87	Joback Method
dvisc	0.0000264	Pa×s	886.48	Joback Method
dvisc	0.0000185	Pa×s	962.10	Joback Method
dvisc	0.0000136	Pa×s	1037.71	Joback Method
dvisc	0.0000104	Pa×s	1113.32	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376775&Units=SI

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