Glutaric acid, 2-bromobenzyl tridecyl ester

Inchi: InChI=1S/C25H39BrO4/c1-2-3-4-5-6-7-8-9-10-11-14-20-29-24(27)18-15-19-25(28)30-21-
InchiKey: QMUUERLXKJOKAL-UHFFFAOYSA-N
Formula: C25H39BrO4
SMILES: CCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccccc1Br
Mol. weight [g/mol]: 483.48

Physical Properties

Property code	Value	Unit	Source
gf	-191.12	kJ/mol	Joback Method
hf	-797.54	kJ/mol	Joback Method
hfus	65.02	kJ/mol	Joback Method
hvap	98.93	kJ/mol	Joback Method
log10ws	-8.77		Crippen Method
logp	7.517		Crippen Method
mcvol	371.730	ml/mol	McGowan Method
pc	1013.59	kPa	Joback Method
rinpol	3294.00		NIST Webbook
rinpol	3294.00		NIST Webbook
tb	1021.80	K	Joback Method
tc	1251.48	K	Joback Method
tf	614.57	K	Joback Method
vc	1.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1221.24	J/mol×K	1021.80	Joback Method
cpg	1285.57	J/mol×K	1213.20	Joback Method
cpg	1275.36	J/mol×K	1174.92	Joback Method
cpg	1263.89	J/mol×K	1136.64	Joback Method
cpg	1251.09	J/mol×K	1098.36	Joback Method
cpg	1236.89	J/mol×K	1060.08	Joback Method
cpg	1294.58	J/mol×K	1251.48	Joback Method
dvisc	0.0000198	Pa×s	1021.80	Joback Method

dvisc	0.0000256	Pa×s	953.93	Joback Method
dvisc	0.0000344	Pa×s	886.06	Joback Method
dvisc	0.0000485	Pa×s	818.18	Joback Method
dvisc	0.0000727	Pa×s	750.31	Joback Method
dvisc	0.0001182	Pa×s	682.44	Joback Method
dvisc	0.0002140	Pa×s	614.57	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=U376771&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