Glutaric acid, 2-bromobenzyl hexadecyl ester

Inchi: InChI=1S/C28H45BrO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-23-32-27(30)21-18-22-28(
InchiKey: XLBATZQUIPEMGK-UHFFFAOYSA-N
Formula: C28H45BrO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccccc1Br
Mol. weight [g/mol]: 525.56

Physical Properties

Property code	Value	Unit	Source
gf	-165.86	kJ/mol	Joback Method
hf	-859.46	kJ/mol	Joback Method
hfus	72.79	kJ/mol	Joback Method
hvap	105.61	kJ/mol	Joback Method
log10ws	-10.03		Crippen Method
logp	8.687		Crippen Method
mcvol	414.000	ml/mol	McGowan Method
pc	850.48	kPa	Joback Method
rinpol	3613.00		NIST Webbook
rinpol	3613.00		NIST Webbook
tb	1090.44	K	Joback Method
tc	1344.26	K	Joback Method
tf	648.38	K	Joback Method
vc	1.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1408.55	J/mol×K	1090.44	Joback Method
cpg	1475.23	J/mol×K	1301.96	Joback Method
cpg	1465.03	J/mol×K	1259.65	Joback Method
cpg	1453.37	J/mol×K	1217.35	Joback Method
cpg	1440.14	J/mol×K	1175.05	Joback Method
cpg	1425.23	J/mol×K	1132.74	Joback Method
cpg	1484.05	J/mol×K	1344.26	Joback Method
dvisc	0.0000123	Pa×s	1090.44	Joback Method

dvisc	0.0000159	Pa×s	1016.76	Joback Method
dvisc	0.0000216	Pa×s	943.09	Joback Method
dvisc	0.0000308	Pa×s	869.41	Joback Method
dvisc	0.0000469	Pa×s	795.73	Joback Method
dvisc	0.0000779	Pa×s	722.06	Joback Method
dvisc	0.0001450	Pa×s	648.38	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=U376774&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

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