

Glutaric acid, 2-bromobenzyl undecyl ester

Inchi:	InChI=1S/C23H35BrO4/c1-2-3-4-5-6-7-8-9-12-18-27-22(25)16-13-17-23(26)28-19-20-14
InchiKey:	ZXIFUBUHYMFNOM-UHFFFAOYSA-N
Formula:	C23H35BrO4
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OCc1ccccc1Br
Mol. weight [g/mol]:	455.43

Physical Properties

Property code	Value	Unit	Source
gf	-207.96	kJ/mol	Joback Method
hf	-756.26	kJ/mol	Joback Method
hfus	59.84	kJ/mol	Joback Method
hvap	94.48	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	6.737		Crippen Method
mvol	343.550	ml/mol	McGowan Method
pc	1149.87	kPa	Joback Method
rinpol	3080.00		NIST Webbook
rinpol	3080.00		NIST Webbook
tb	976.04	K	Joback Method
tc	1195.50	K	Joback Method
tf	592.03	K	Joback Method
vc	1.325	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1098.41	J/molxK	976.04	Joback Method
cpg	1113.53	J/molxK	1012.62	Joback Method
cpg	1127.34	J/molxK	1049.19	Joback Method
cpg	1139.90	J/molxK	1085.77	Joback Method
cpg	1151.24	J/molxK	1122.35	Joback Method
cpg	1161.43	J/molxK	1158.93	Joback Method
cpg	1170.51	J/molxK	1195.50	Joback Method
dvisc	0.0002740	Paxs	592.03	Joback Method

dvisc	0.0001544	Paxs	656.03	Joback Method
dvisc	0.0000964	Paxs	720.03	Joback Method
dvisc	0.0000650	Paxs	784.03	Joback Method
dvisc	0.0000465	Paxs	848.04	Joback Method
dvisc	0.0000348	Paxs	912.04	Joback Method
dvisc	0.0000271	Paxs	976.04	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U376769&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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