

Glutaric acid, 2-bromo-5-fluorobenzyl decyl ester

Inchi:	InChI=1S/C22H32BrFO4/c1-2-3-4-5-6-7-8-9-15-27-21(25)11-10-12-22(26)28-17-18-16-1
InchiKey:	FEOVHAHXKWUQLB-UHFFFAOYSA-N
Formula:	C22H32BrFO4
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OCc1cc(F)ccc1Br
Mol. weight [g/mol]:	459.39

Physical Properties

Property code	Value	Unit	Source
gf	-420.82	kJ/mol	Joback Method
hf	-943.20	kJ/mol	Joback Method
hfus	59.94	kJ/mol	Joback Method
hvap	92.10	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	6.486		Crippen Method
mvol	331.230	ml/mol	McGowan Method
pc	1178.47	kPa	Joback Method
rmpol	2925.00		NIST Webbook
rmpol	2925.00		NIST Webbook
tb	957.41	K	Joback Method
tc	1172.78	K	Joback Method
tf	593.87	K	Joback Method
vc	1.288	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1043.77	J/molxK	957.41	Joback Method
cpg	1058.33	J/molxK	993.31	Joback Method
cpg	1071.63	J/molxK	1029.20	Joback Method
cpg	1083.72	J/molxK	1065.10	Joback Method
cpg	1094.64	J/molxK	1100.99	Joback Method
cpg	1104.41	J/molxK	1136.89	Joback Method
cpg	1113.09	J/molxK	1172.78	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=U377069&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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