

Glutaric acid, 2,6-difluoro-4-bromobenzyl undecyl ester

Inchi:	InChI=1S/C23H33BrF2O4/c1-2-3-4-5-6-7-8-9-10-14-29-22(27)12-11-13-23(28)30-17-19-
InchiKey:	QTVKJUDZWNXNJK-UHFFFAOYSA-N
Formula:	C23H33BrF2O4
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]:	491.41

Physical Properties

Property code	Value	Unit	Source
gf	-616.84	kJ/mol	Joback Method
hf	-1171.42	kJ/mol	Joback Method
hfus	65.22	kJ/mol	Joback Method
hvap	94.17	kJ/mol	Joback Method
log10ws	-8.60		Crippen Method
logp	7.015		Crippen Method
mcvol	347.090	ml/mol	McGowan Method
pc	1061.71	kPa	Joback Method
rinqol	2999.00		NIST Webbook
tb	984.54	K	Joback Method
tc	1205.68	K	Joback Method
tf	618.25	K	Joback Method
vc	1.361	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1110.23	J/molxK	984.54	Joback Method
cpg	1124.83	J/molxK	1021.40	Joback Method
cpg	1138.07	J/molxK	1058.25	Joback Method
cpg	1149.98	J/molxK	1095.11	Joback Method
cpg	1160.61	J/molxK	1131.97	Joback Method
cpg	1170.00	J/molxK	1168.82	Joback Method
cpg	1178.18	J/molxK	1205.68	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=U376827&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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