

Sebacic acid, 2-bromo-5-fluorobenzyl hexyl ester

Inchi:	InChI=1S/C23H34BrFO4/c1-2-3-4-11-16-28-22(26)12-9-7-5-6-8-10-13-23(27)29-18-19-1
InchiKey:	FSBVBZVQAMBYNT-UHFFFAOYSA-N
Formula:	C23H34BrFO4
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)OCc1cc(F)ccc1Br
Mol. weight [g/mol]:	473.42

Physical Properties

Property code	Value	Unit	Source
gf	-412.40	kJ/mol	Joback Method
hf	-963.84	kJ/mol	Joback Method
hfus	62.53	kJ/mol	Joback Method
hvap	94.32	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	6.876		Crippen Method
mvol	345.320	ml/mol	McGowan Method
pc	1104.47	kPa	Joback Method
rmpol	3004.00		NIST Webbook
rmpol	3004.00		NIST Webbook
tb	980.29	K	Joback Method
tc	1200.16	K	Joback Method
tf	605.14	K	Joback Method
vc	1.343	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.35	J/molxK	980.29	Joback Method
cpg	1119.18	J/molxK	1016.93	Joback Method
cpg	1132.69	J/molxK	1053.58	Joback Method
cpg	1144.91	J/molxK	1090.22	Joback Method
cpg	1155.89	J/molxK	1126.87	Joback Method
cpg	1165.67	J/molxK	1163.51	Joback Method
cpg	1174.31	J/molxK	1200.16	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=U380681&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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