

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

Inchi:	InChI=1S/C21H30BrFO4/c1-2-3-14-26-20(24)10-8-6-4-5-7-9-11-21(25)27-16-17-15-18(2
InchiKey:	VKYAZXYGLVZYTC-UHFFFAOYSA-N
Formula:	C21H30BrFO4
SMILES:	CCCCOC(=O)CCCCCCCC(=O)OCc1cc(F)ccc1Br
Mol. weight [g/mol]:	445.36

Physical Properties

Property code	Value	Unit	Source
gf	-429.24	kJ/mol	Joback Method
hf	-922.56	kJ/mol	Joback Method
hfus	57.35	kJ/mol	Joback Method
hvap	89.87	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.096		Crippen Method
mvol	317.140	ml/mol	McGowan Method
pc	1260.16	kPa	Joback Method
rinpol	2817.00		NIST Webbook
rinpol	2817.00		NIST Webbook
tb	934.53	K	Joback Method
tc	1146.38	K	Joback Method
tf	582.60	K	Joback Method
vc	1.232	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.74	J/molxK	934.53	Joback Method
cpg	998.04	J/molxK	969.84	Joback Method
cpg	1011.15	J/molxK	1005.15	Joback Method
cpg	1023.11	J/molxK	1040.46	Joback Method
cpg	1033.94	J/molxK	1075.77	Joback Method
cpg	1043.69	J/molxK	1111.07	Joback Method
cpg	1052.38	J/molxK	1146.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380679&Units=SI
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

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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