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

Inchi: InChI=1S/C25H38BrFO4/c1-2-3-4-5-10-13-18-30-24(28)14-11-8-6-7-9-12-15-25(29)31-2(

InchiKey: FPYFJYLZOHVXHY-UHFFFAOYSA-N

Formula: C25H38BrFO4

SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1cc(F)ccc1Br

Mol. weight [g/mol]: 501.47

Physical Properties

Property code	Value	Unit	Source
gf	-395.56	kJ/mol	Joback Method
hf	-1005.12	kJ/mol	Joback Method
hfus	67.71	kJ/mol	Joback Method
hvap	98.77	kJ/mol	Joback Method
log10ws	-9.11		Crippen Method
logp	7.656		Crippen Method
mcvol	373.500	ml/mol	McGowan Method
pc	975.95	kPa	Joback Method
rinpol	3198.00		NIST Webbook
rinpol	3198.00		NIST Webbook
tb	1026.05	K	Joback Method
tc	1258.11	K	Joback Method
tf	627.68	K	Joback Method
vc	1.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1226.96	J/mol×K	1026.05	Joback Method
cpg	1242.40	J/mol×K	1064.73	Joback Method
cpg	1256.33	J/mol×K	1103.40	Joback Method
cpg	1268.81	J/mol×K	1142.08	Joback Method
cpg	1279.90	J/mol×K	1180.76	Joback Method
cpg	1289.65	J/mol×K	1219.44	Joback Method
cpg	1298.13	J/mol×K	1258.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380683&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume