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

Inchi: InChI=1S/C24H36BrFO4/c1-2-3-4-9-12-17-29-23(27)13-10-7-5-6-8-11-14-24(28)30-19-2

InchiKey: AUANCSPFXOYJIM-UHFFFAOYSA-N

Formula: C24H36BrFO4

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

Mol. weight [g/mol]: 487.44

Physical Properties

Property code	Value	Unit	Source
gf	-403.98	kJ/mol	Joback Method
hf	-984.48	kJ/mol	Joback Method
hfus	65.12	kJ/mol	Joback Method
hvap	96.55	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	7.266		Crippen Method
mcvol	359.410	ml/mol	McGowan Method
pc	1037.23	kPa	Joback Method
rinpol	3099.00		NIST Webbook
rinpol	3099.00		NIST Webbook
tb	1003.17	K	Joback Method
tc	1228.58	K	Joback Method
tf	616.41	K	Joback Method
vc	1.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1165.43	J/mol×K	1003.17	Joback Method
cpg	1180.55	J/mol×K	1040.74	Joback Method
cpg	1194.27	J/mol×K	1078.31	Joback Method
cpg	1206.62	J/mol×K	1115.87	Joback Method
cpg	1217.65	J/mol×K	1153.44	Joback Method
cpg	1227.43	J/mol×K	1191.01	Joback Method
cpg	1236.00	J/mol×K	1228.58	Joback Method

Sources

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=U380682&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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