Sebacic acid, 2-bromo-4-fluorophenyl decyl ester

Inchi: InChI=1S/C26H40BrFO4/c1-2-3-4-5-6-9-12-15-20-31-25(29)16-13-10-7-8-11-14-17-26(3

InchiKey: XBMTWJKHTFAEFR-UHFFFAOYSA-N

Formula: C26H40BrFO4

SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 515.50

Physical Properties

Property code	Value	Unit	Source
gf	-387.14	kJ/mol	Joback Method
hf	-1025.76	kJ/mol	Joback Method
hfus	70.30	kJ/mol	Joback Method
hvap	101.00	kJ/mol	Joback Method
log10ws	-9.68		Crippen Method
logp	8.298		Crippen Method
mcvol	387.590	ml/mol	McGowan Method
pc	919.95	kPa	Joback Method
rinpol	3411.00		NIST Webbook
tb	1048.93	K	Joback Method
tc	1288.85	K	Joback Method
tf	638.95	K	Joback Method
vc	1.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1288.90	J/mol×K	1048.93	Joback Method
cpg	1304.69	J/mol×K	1088.92	Joback Method
cpg	1318.85	J/mol×K	1128.90	Joback Method
cpg	1331.45	J/mol×K	1168.89	Joback Method
cpg	1342.57	J/mol×K	1208.88	Joback Method
cpg	1352.28	J/mol×K	1248.87	Joback Method
cpg	1360.64	J/mol×K	1288.85	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=U354559&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume