Sebacic acid, 4-bromo-2,6-difluorobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C24H35BrF2O4/c1-4-11-22(17(2)3)31-24(29)13-10-8-6-5-7-9-12-23(28)30-16-
InchiKey: IDRNHHMDAQAFEU-UHFFFAOYSA-N
Formula: C24H35BrF2O4
SMILES: CCCC(OC(=O)CCCCCCCCC(=O)OCc1c(F)cc(Br)cc1F)C(C)C
Mol. weight [g/mol]: 505.43

Physical Properties

Property code	Value	Unit	Source
gf	-613.30	kJ/mol	Joback Method
hf	-1202.62	kJ/mol	Joback Method
hfus	60.76	kJ/mol	Joback Method
hvap	95.62	kJ/mol	Joback Method
log10ws	-8.89		Crippen Method
logp	7.259		Crippen Method
mcvol	361.180	ml/mol	McGowan Method
pc	1008.45	kPa	Joback Method
rinpol	2930.00		NIST Webbook
rinpol	2930.00		NIST Webbook
tb	1006.54	K	Joback Method
tc	1232.84	K	Joback Method
tf	599.52	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1171.89	J/mol×K	1006.54	Joback Method
cpg	1186.60	J/mol×K	1044.26	Joback Method
cpg	1199.84	J/mol×K	1081.97	Joback Method
cpg	1211.64	J/mol×K	1119.69	Joback Method
cpg	1222.06	J/mol×K	1157.41	Joback Method
cpg	1231.14	J/mol×K	1195.13	Joback Method
cpg	1238.92	J/mol×K	1232.84	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=U380809&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