Sebacic acid, 4-bromo-2,6-difluorobenzyl nonyl ester

Inchi: InChI=1S/C26H39BrF2O4/c1-2-3-4-5-8-11-14-17-32-25(30)15-12-9-6-7-10-13-16-26(31)

InchiKey: QQDUHMDHNJCXSP-UHFFFAOYSA-N

Formula: C26H39BrF2O4

SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1c(F)cc(Br)cc1F

Mol. weight [g/mol]: 533.49

Physical Properties

Property code	Value	Unit	Source
gf	-591.58	kJ/mol	Joback Method
hf	-1233.34	kJ/mol	Joback Method
hfus	72.99	kJ/mol	Joback Method
hvap	100.84	kJ/mol	Joback Method
log10ws	-9.86		Crippen Method
logp	8.185		Crippen Method
mcvol	389.360	ml/mol	McGowan Method
pc	887.35	kPa	Joback Method
rinpol	3235.00		NIST Webbook
rinpol	3235.00		NIST Webbook
tb	1053.18	K	Joback Method
tc	1297.53	K	Joback Method
tf	652.06	K	Joback Method
vc	1.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1294.44	J/mol×K	1053.18	Joback Method
cpg	1310.09	J/mol×K	1093.91	Joback Method
cpg	1324.02	J/mol×K	1134.63	Joback Method
cpg	1336.29	J/mol×K	1175.36	Joback Method
cpg	1346.99	J/mol×K	1216.08	Joback Method
cpg	1356.16	J/mol×K	1256.81	Joback Method
cpg	1363.88	J/mol×K	1297.53	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=U380813&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