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

Inchi: InChI=1S/C24H35BrF2O4/c1-2-3-4-9-12-15-30-23(28)13-10-7-5-6-8-11-14-24(29)31-18-

InchiKey: PVGUGPLPLUTPJQ-UHFFFAOYSA-N

Formula: C24H35BrF2O4

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

Mol. weight [g/mol]: 505.43

Physical Properties

Property code	Value	Unit	Source
gf	-608.42	kJ/mol	Joback Method
hf	-1192.06	kJ/mol	Joback Method
hfus	67.81	kJ/mol	Joback Method
hvap	96.39	kJ/mol	Joback Method
log10ws	-9.02		Crippen Method
logp	7.405		Crippen Method
mcvol	361.180	ml/mol	McGowan Method
pc	998.28	kPa	Joback Method
rinpol	3053.00		NIST Webbook
rinpol	3053.00		NIST Webbook
tb	1007.42	K	Joback Method
tc	1235.09	K	Joback Method
tf	629.52	K	Joback Method
vc	1.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1171.21	J/mol×K	1007.42	Joback Method
cpg	1186.14	J/mol×K	1045.37	Joback Method
cpg	1199.60	J/mol×K	1083.31	Joback Method
cpg	1211.64	J/mol×K	1121.26	Joback Method
cpg	1222.31	J/mol×K	1159.20	Joback Method
cpg	1231.66	J/mol×K	1197.15	Joback Method
cpg	1239.73	J/mol×K	1235.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380811&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