

Succinic acid, 4-bromo-2,6-difluorobenzyl tridecyl ester

Inchi:	InChI=1S/C24H35BrF2O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-30-23(28)13-14-24(29)31-18-
InchiKey:	LVIQFUQQCIYLAN-UHFFFAOYSA-N
Formula:	C24H35BrF2O4
SMILES:	CCCCCCCCCCCCOC(=O)CCC(=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
mvol	361.180	ml/mol	McGowan Method
pc	998.28	kPa	Joback Method
rinpol	3050.00		NIST Webbook
rinpol	3050.00		NIST Webbook
tb	1007.42	K	Joback Method
tc	1235.09	K	Joback Method
tf	629.52	K	Joback Method
vc	1.417	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U381164&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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