2,4-Difluorobenzoic acid, nonadecyl ester

Inchi: InChI=1S/C26H42F2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-30-26(29)24
InchiKey: SBGXAPGVTQOVQD-UHFFFAOYSA-N
Formula: C26H42F2O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 424.61

Physical Properties

Property code	Value	Unit	Source
gf	-362.35	kJ/mol	Joback Method
hf	-1003.40	kJ/mol	Joback Method
hfus	65.31	kJ/mol	Joback Method
hvap	84.59	kJ/mol	Joback Method
log10ws	-9.91		Crippen Method
logp	8.773		Crippen Method
mcvol	364.420	ml/mol	McGowan Method
pc	836.76	kPa	Joback Method
rinpol	2897.00		NIST Webbook
rinpol	2897.00		NIST Webbook
tb	905.75	K	Joback Method
tc	1109.25	K	Joback Method
tf	507.58	K	Joback Method
vc	1.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1206.66	J/mol×K	905.75	Joback Method
cpg	1226.19	J/mol×K	939.67	Joback Method
cpg	1244.42	J/mol×K	973.58	Joback Method
cpg	1261.40	J/mol×K	1007.50	Joback Method
cpg	1277.17	J/mol×K	1041.42	Joback Method
cpg	1291.80	J/mol×K	1075.34	Joback Method
cpg	1305.33	J/mol×K	1109.25	Joback Method

Sources

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=U338797&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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