3,4-Difluorobenzoic acid, tridecyl ester

Inchi: InChI=1S/C20H30F2O2/c1-2-3-4-5-6-7-8-9-10-11-12-15-24-20(23)17-13-14-18(21)19(22
InchiKey: BECRBFJRQSXZLS-UHFFFAOYSA-N
Formula: C20H30F2O2
SMILES: CCCCCCCCCCCCCOC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 340.45

Physical Properties

Property code	Value	Unit	Source
gf	-412.87	kJ/mol	Joback Method
hf	-879.56	kJ/mol	Joback Method
hfus	49.77	kJ/mol	Joback Method
hvap	71.24	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	6.433		Crippen Method
mcvol	279.880	ml/mol	McGowan Method
pc	1204.80	kPa	Joback Method
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
tb	768.47	K	Joback Method
tc	951.81	K	Joback Method
tf	439.96	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.97	J/mol×K	768.47	Joback Method
cpg	858.07	J/mol×K	799.03	Joback Method
cpg	874.22	J/mol×K	829.58	Joback Method
cpg	889.46	J/mol×K	860.14	Joback Method
cpg	903.80	J/mol×K	890.70	Joback Method
cpg	917.28	J/mol×K	921.25	Joback Method
cpg	929.92	J/mol×K	951.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338869&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

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

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