3,4-Difluorobenzoic acid, 7-tridecyl ester

Inchi: InChI=1S/C20H30F2O2/c1-3-5-7-9-11-17(12-10-8-6-4-2)24-20(23)16-13-14-18(21)19(22
InchiKey: YJCZOQSDYFVPEL-UHFFFAOYSA-N
Formula: C20H30F2O2
SMILES: CCCCCCC(CCCCCC)OC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 340.45

Physical Properties

Property code	Value	Unit	Source
gf	-415.31	kJ/mol	Joback Method
hf	-884.84	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	70.85	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	6.431		Crippen Method
mcvol	279.880	ml/mol	McGowan Method
pc	1211.51	kPa	Joback Method
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
tb	768.03	K	Joback Method
tc	953.00	K	Joback Method
tf	424.96	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.47	J/mol×K	768.03	Joback Method
cpg	858.73	J/mol×K	798.86	Joback Method
cpg	875.02	J/mol×K	829.69	Joback Method
cpg	890.36	J/mol×K	860.52	Joback Method
cpg	904.80	J/mol×K	891.34	Joback Method
cpg	918.34	J/mol×K	922.17	Joback Method
cpg	931.02	J/mol×K	953.00	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=U338604&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

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