3,4-Difluorobenzoic acid, dodecyl ester

Inchi: InChI=1S/C19H28F2O2/c1-2-3-4-5-6-7-8-9-10-11-14-23-19(22)16-12-13-17(20)18(21)15
InchiKey: YIFWZXZTDAWGGQ-UHFFFAOYSA-N
Formula: C19H28F2O2
SMILES: CCCCCCCCCCCCOC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 326.42

Physical Properties

Property code	Value	Unit	Source
gf	-421.29	kJ/mol	Joback Method
hf	-858.92	kJ/mol	Joback Method
hfus	47.18	kJ/mol	Joback Method
hvap	69.01	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	6.043		Crippen Method
mcvol	265.790	ml/mol	McGowan Method
pc	1289.29	kPa	Joback Method
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook
tb	745.59	K	Joback Method
tc	928.10	K	Joback Method
tf	428.69	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.92	J/mol×K	745.59	Joback Method
cpg	799.66	J/mol×K	776.01	Joback Method
cpg	815.50	J/mol×K	806.43	Joback Method
cpg	830.46	J/mol×K	836.85	Joback Method
cpg	844.56	J/mol×K	867.26	Joback Method
cpg	857.82	J/mol×K	897.68	Joback Method
cpg	870.27	J/mol×K	928.10	Joback Method

Sources

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=U338868&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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