2,4-Difluorobenzoic acid, 4-pentadecyl ester

Inchi: InChI=1S/C22H34F2O2/c1-3-5-6-7-8-9-10-11-12-14-19(13-4-2)26-22(25)20-16-15-18(23
InchiKey: QLUNNPIWVXFGLI-UHFFFAOYSA-N
Formula: C22H34F2O2
SMILES: CCCCCCCCCCCC(CCC)OC(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 368.50

Physical Properties

Property code	Value	Unit	Source
gf	-398.47	kJ/mol	Joback Method
hf	-926.12	kJ/mol	Joback Method
hfus	51.42	kJ/mol	Joback Method
hvap	75.30	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	7.211		Crippen Method
mcvol	308.060	ml/mol	McGowan Method
pc	1064.48	kPa	Joback Method
rinpol	2332.00		NIST Webbook
rinpol	2332.00		NIST Webbook
tb	813.79	K	Joback Method
tc	1001.75	K	Joback Method
tf	447.50	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	960.31	J/mol×K	813.79	Joback Method
cpg	978.23	J/mol×K	845.12	Joback Method
cpg	995.09	J/mol×K	876.44	Joback Method
cpg	1010.93	J/mol×K	907.77	Joback Method
cpg	1025.77	J/mol×K	939.09	Joback Method
cpg	1039.66	J/mol×K	970.42	Joback Method
cpg	1052.62	J/mol×K	1001.75	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=U338578&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

Latest version available from:

https://www.chemeo.com/cid/124-414-4/2-4-Difluorobenzoic-acid-4-pentadecyl-ester.pdf

Generated by Cheméo on 2024-10-12 09:17:17.237941093 +0000 UTC m=+3305499.874910341.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.