2,6-Difluoro-3-methylbenzoic acid, cyclohexylmethyl ester

Inchi: InChI=1S/C15H18F2O2/c1-10-7-8-12(16)13(14(10)17)15(18)19-9-11-5-3-2-4-6-11/h7-8,1

InchiKey: XQVMNPOCUMAMCH-UHFFFAOYSA-N

Formula: C15H18F2O2

SMILES: Cc1ccc(F)c(C(=O)OCC2CCCCC2)c1F

Mol. weight [g/mol]: 268.30

Physical Properties

Property code	Value	Unit	Source
gf	-440.15	kJ/mol	Joback Method
hf	-733.51	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	61.20	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.010		Crippen Method
mcvol	198.570	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	1876.00		NIST Webbook
rinpol	1876.00		NIST Webbook
tb	678.60	K	Joback Method
tc	891.98	K	Joback Method
tf	403.51	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.81	J/mol×K	678.60	Joback Method
cpg	571.26	J/mol×K	714.16	Joback Method
cpg	587.58	J/mol×K	749.73	Joback Method
cpg	602.79	J/mol×K	785.29	Joback Method
cpg	616.92	J/mol×K	820.85	Joback Method
cpg	629.98	J/mol×K	856.42	Joback Method
cpg	641.99	J/mol×K	891.98	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=U357680&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