2,6-Difluorobenzoic acid, 2-naphthyl ester

Inchi: InChI=1S/C17H10F2O2/c18-14-6-3-7-15(19)16(14)17(20)21-13-9-8-11-4-1-2-5-12(11)10
InchiKey: PMPDADBYVZJXAX-UHFFFAOYSA-N
Formula: C17H10F2O2
SMILES: O=C(Oc1ccc2ccccc2c1)c1c(F)cccc1F
Mol. weight [g/mol]: 284.26

Physical Properties

Property code	Value	Unit	Source
gf	-228.70	kJ/mol	Joback Method
hf	-401.51	kJ/mol	Joback Method
hfus	32.67	kJ/mol	Joback Method
hvap	69.14	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	4.337		Crippen Method
mcvol	194.390	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook
tb	750.47	K	Joback Method
tc	987.06	K	Joback Method
tf	477.79	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.13	J/mol×K	750.47	Joback Method
cpg	528.91	J/mol×K	789.90	Joback Method
cpg	540.65	J/mol×K	829.33	Joback Method
cpg	551.41	J/mol×K	868.77	Joback Method
cpg	561.26	J/mol×K	908.20	Joback Method
cpg	570.27	J/mol×K	947.63	Joback Method
cpg	578.53	J/mol×K	987.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307563&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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