Benzoic acid, 4-fluoro-, 2-naphtyl ester

Other names: 4-Fluorobenzoic acid, 2-naphthyl ester
Inchi: InChI=1S/C17H11FO2/c18-15-8-5-13(6-9-15)17(19)20-16-10-7-12-3-1-2-4-14(12)11-16/h
InchiKey: XFEWKHXRJAPWJI-UHFFFAOYSA-N
Formula: C17H11FO2
SMILES: O=C(Oc1ccc2ccccc2c1)c1ccc(F)cc1
Mol. weight [g/mol]: 266.27
CAS: 90172-41-1

Physical Properties

Property code	Value	Unit	Source
gf	-24.26	kJ/mol	Joback Method
hf	-193.93	kJ/mol	Joback Method
hfus	29.98	kJ/mol	Joback Method
hvap	69.29	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	4.198		Crippen Method
mcvol	192.620	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	746.22	K	Joback Method
tc	992.54	K	Joback Method
tf	464.68	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.71	J/mol×K	746.22	Joback Method
cpg	523.29	J/mol×K	787.27	Joback Method
cpg	535.71	J/mol×K	828.33	Joback Method
cpg	547.05	J/mol×K	869.38	Joback Method
cpg	557.42	J/mol×K	910.43	Joback Method
cpg	566.89	J/mol×K	951.48	Joback Method

cpg	575.55	J/mol×K	992.54	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=C90172411&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