Fumaric acid, naphth-2-yl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C17H12F4O4/c18-16(19)17(20,21)10-24-14(22)7-8-15(23)25-13-6-5-11-3-1-2-

InchiKey: NXATWHFSNAFXCX-BQYQJAHWSA-N

Formula: C17H12F4O4

SMILES: O=C(C=CC(=O)Oc1ccc2ccccc2c1)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 356.27

Physical Properties

Property code	Value	Unit	Source
gf	-864.77	kJ/mol	Joback Method
hf	-1148.93	kJ/mol	Joback Method
hfus	37.62	kJ/mol	Joback Method
hvap	71.33	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	3.745		Crippen Method
mcvol	224.830	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinpol	2207.00		NIST Webbook
rinpol	2207.00		NIST Webbook
tb	789.15	K	Joback Method
tc	997.56	K	Joback Method
tf	482.01	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.79	J/mol×K	789.15	Joback Method
cpg	652.29	J/mol×K	823.89	Joback Method
cpg	662.93	J/mol×K	858.62	Joback Method
cpg	672.77	J/mol×K	893.36	Joback Method
cpg	681.88	J/mol×K	928.09	Joback Method
cpg	690.35	J/mol×K	962.83	Joback Method
cpg	698.24	J/mol×K	997.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405822&Units=SI

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