1-Naphthaleneacetic acid, 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C15H12F4O2/c16-14(17)15(18,19)9-21-13(20)8-11-6-3-5-10-4-1-2-7-12(10)11

InchiKey: BNRXXMNOZGOCRS-UHFFFAOYSA-N

Formula: C15H12F4O2

SMILES: O=C(Cc1cccc2ccccc12)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 300.25

Physical Properties

Property code	Value	Unit	Source
gf	-727.91	kJ/mol	Joback Method
hf	-980.07	kJ/mol	Joback Method
hfus	29.45	kJ/mol	Joback Method
hvap	57.77	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.826		Crippen Method
mcvol	193.510	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	2159.00		NIST Webbook
tb	662.94	K	Joback Method
tc	863.79	K	Joback Method
tf	392.39	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.45	J/mol×K	662.94	Joback Method
cpg	533.72	J/mol×K	696.42	Joback Method
cpg	546.04	J/mol×K	729.89	Joback Method
cpg	557.49	J/mol×K	763.37	Joback Method
cpg	568.11	J/mol×K	796.84	Joback Method
cpg	577.98	J/mol×K	830.32	Joback Method
cpg	587.15	J/mol×K	863.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415041&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