1-Naphthaleneacetic acid, 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C15H13F3O2/c1-10(15(16,17)18)20-14(19)9-12-7-4-6-11-5-2-3-8-13(11)12/h2-

InchiKey: PBMHWLLUYZBYCZ-UHFFFAOYSA-N

Formula: C15H13F3O2

SMILES: CC(OC(=O)Cc1cccc2ccccc12)C(F)(F)F

Mol. weight [g/mol]: 282.26

Physical Properties

Property code	Value	Unit	Source
gf	-533.10	kJ/mol	Joback Method
hf	-783.96	kJ/mol	Joback Method
hfus	26.37	kJ/mol	Joback Method
hvap	58.58	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.876		Crippen Method
mcvol	191.740	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	2140.00		NIST Webbook
rinpol	2140.00		NIST Webbook
tb	663.67	K	Joback Method
tc	873.06	K	Joback Method
tf	391.80	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.43	J/mol×K	663.67	Joback Method
cpg	526.32	J/mol×K	698.57	Joback Method
cpg	539.19	J/mol×K	733.47	Joback Method
cpg	551.12	J/mol×K	768.37	Joback Method
cpg	562.19	J/mol×K	803.27	Joback Method
cpg	572.45	J/mol×K	838.16	Joback Method
cpg	581.98	J/mol×K	873.06	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=U415040&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