Trifluoroacetic acid, 2-naphthyl ester

Other names:	2-Naphthol, TFA
	2-Naphthol, trifluoroacetate
Inchi:	InChI=1S/C12H7F3O2/c13-12(14,15)11(16)17-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H
InchiKey:	FBGJNOFLJYQIDX-UHFFFAOYSA-N
Formula:	C12H7F3O2
SMILES:	O=C(Oc1ccc2ccccc2c1)C(F)(F)F
Mol. weight [g/mol]:	240.18

Physical Properties

Property code	Value	Unit	Source
gf	-555.92	kJ/mol	Joback Method
hf	-716.76	kJ/mol	Joback Method
hfus	22.12	kJ/mol	Joback Method
hvap	52.29	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.308		Crippen Method
mcvol	149.470	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	1341.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1346.00		NIST Webbook
tb	595.47	K	Joback Method
tc	811.04	K	Joback Method
tf	372.99	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.86	J/mol×K	595.47	Joback Method
cpg	376.83	J/mol×K	631.40	Joback Method
cpg	387.85	J/mol×K	667.33	Joback Method
cpg	397.97	J/mol×K	703.25	Joback Method
cpg	407.28	J/mol×K	739.18	Joback Method

cpg	415.82	J/mol×K	775.11	Joback Method
cpg	423.68	J/mol×K	811.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307657&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

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

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