

Trifluoroacetoacetyl-2-naphthalene

Other names:	1,3-Butanedione, 4,4,4-trifluoro-1-(2-naphthalenyl)- 1,3-Butanedione, 4,4,4-trifluoro-1-(2-naphthyl)- 2-(4,4,4-Trifluoro-1,3-dioxobutyl)naphthalene 4,4,4-Trifluoro-1-(2-naphthyl)-butan-1,3-dione
Inchi:	InChI=1S/C14H9F3O2/c15-14(16,17)13(19)8-12(18)11-6-5-9-3-1-2-4-10(9)7-11/h1-7H,8H
InchiKey:	WVVLURYIQCXPIV-UHFFFAOYSA-N
Formula:	C14H9F3O2
SMILES:	O=C(CC(=O)C(F)(F)F)c1ccc2ccccc2c1
Mol. weight [g/mol]:	266.22
CAS:	893-33-4

Physical Properties

Property code	Value	Unit	Source
gf	-563.00	kJ/mol	Joback Method
hf	-738.40	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hsub	108.70 ± 0.60	kJ/mol	NIST Webbook
hvap	61.08	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	3.544		Crippen Method
mcvol	173.350	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
tb	672.68	K	Joback Method
tc	890.20	K	Joback Method
tf	423.23	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.12	J/mol×K	672.68	Joback Method
cpg	462.90	J/mol×K	708.93	Joback Method
cpg	473.72	J/mol×K	745.19	Joback Method
cpg	483.67	J/mol×K	781.44	Joback Method

cpg	492.82	J/mol×K	817.69	Joback Method
cpg	501.27	J/mol×K	853.95	Joback Method
cpg	509.10	J/mol×K	890.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C893334&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
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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