2-(4,4,4-TRIFLUORO-1,3-DIOXOBUTYL)NAPHTHA

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

Physical Properties

Property code	Value	Unit	Source
hf	-801.51	kJ/mol	Cheméo Relay (1.0)
hfus	27.71	kJ/mol	Joback Method
hsub	108.70 ± 0.60	kJ/mol	NIST Webbook
ie	8.35	eV	Cheméo Relay (1.0)
logp	3.544		Crippen Method
mcvol	173.350	ml/mol	McGowan Method
tb	594.31	K	Cheméo Relay (1.0)
tf	346.87	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C893334&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point