2,7-DIACETYL-9-FLUORENONE

Inchi: InChI=1S/C17H12O3/c1-9(18)11-3-5-13-14-6-4-12(10(2)19)8-16(14)17(20)15(13)7-11/h3
InchiKey: LSDGVBCTFOMRGW-UHFFFAOYSA-N
Formula: C17H12O3
SMILES: CC(=O)c1ccc2c(c1)C(=O)c1cc(C(C)=O)ccc1-2
Mol. weight [g/mol]: 264.28

Physical Properties

Property code	Value	Unit	Source
af	0.7510		Cheméo Relay (1.0)
gf	-9.21	kJ/mol	Joback Method
hf	-320.16	kJ/mol	Cheméo Relay (1.0)
hfus	30.28	kJ/mol	Joback Method
hvap	108.82	kJ/mol	Cheméo Relay (1.0)
ie	8.95	eV	Cheméo Relay (1.0)
log10ws	-4.80		Cheméo Relay (1.0)
logp	3.303		Crippen Method
mcvol	196.720	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
tb	674.02	K	Cheméo Relay (1.0)
tc	985.71	K	Cheméo Relay (1.0)
tf	487.58	K	Cheméo Relay (1.0)
vc	0.741	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.97	J/mol×K	840.07	Joback Method
cpg	564.07	J/mol×K	881.74	Joback Method
cpg	575.28	J/mol×K	923.42	Joback Method
cpg	585.69	J/mol×K	965.09	Joback Method
cpg	595.38	J/mol×K	1006.77	Joback Method
cpg	604.43	J/mol×K	1048.44	Joback Method
cpg	612.94	J/mol×K	1090.12	Joback Method

Sources

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=C39665899&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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