

acetyl benzenecarboperoxoate

Inchi:	InChI=1S/C9H8O4/c1-7(10)12-13-9(11)8-5-3-2-4-6-8/h2-6H,1H3
InchiKey:	PDAVOLCVHOKLEO-UHFFFAOYSA-N
Formula:	C9H8O4
SMILES:	CC(=O)OOC(=O)c1ccccc1
Mol. weight [g/mol]:	180.16
CAS:	644-31-5

Physical Properties

Property code	Value	Unit	Source
af	0.6288		Cheméo Relay (1.0)
gf	-483.43	kJ/mol	Joback Method
hf	-400.88	kJ/mol	Cheméo Relay (1.0)
hfus	21.85	kJ/mol	Joback Method
hvap	81.10	kJ/mol	Cheméo Relay (1.0)
ie	9.11	eV	Cheméo Relay (1.0)
log10ws	-2.06		Cheméo Relay (1.0)
logp	1.321		Crippen Method
mcvol	128.790	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
tb	527.88	K	Cheméo Relay (1.0)
tc	722.27	K	Cheméo Relay (1.0)
tf	310.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	0.482	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	1.16200e+01
Coeff. B	6.70320e-01

Coeff. C	-3.07800e-04
Coeff. D	7.20000e-09
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	$Y = \exp(A + B/T + C \cdot \ln(T) + D \cdot T^E)$
Y unit	Pa·s
Coeff. A	-1.22572e+01
Coeff. B	1.97074e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	310.15
Temperature range (K), max.	536.09

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

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>

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

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