

Alphozone

Inchi:	InChI=1S/C8H10O8/c9-5(10)1-3-7(13)15-16-8(14)4-2-6(11)12/h1-4H2,(H,9,10)(H,11,12)
InchiKey:	MKTOIPPVFPJEQO-UHFFFAOYSA-N
Formula:	C8H10O8
SMILES:	O=C(O)CCC(=O)OOC(=O)CCC(=O)O
Mol. weight [g/mol]:	234.16
CAS:	123-23-9

Physical Properties

Property code	Value	Unit	Source
af	1.0688		Cheméo Relay (1.0)
hf	-1313.82	kJ/mol	Cheméo Relay (1.0)
hfus	45.50	kJ/mol	Joback Method
hvap	123.03	kJ/mol	Cheméo Relay (1.0)
ie	10.55	eV	Cheméo Relay (1.0)
log10ws	-0.69		Cheméo Relay (1.0)
logp	-0.283		Crippen Method
mcvol	153.340	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
tb	570.20	K	Cheméo Relay (1.0)
tc	815.26	K	Cheméo Relay (1.0)
tf	400.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	0.594	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	5.56340e+01
Coeff. B	7.55800e-01
Coeff. C	-3.67400e-04

Coeff. D	2.58000e-08
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	-1.36300e+01
Coeff. B	3.38104e+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.	400.15
Temperature range (K), max.	696.96

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):
Joback Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
i_e:	Ionization energy
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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