

7-oxabicyclo[4.1.0]heptan-4-ylmethyl
7-oxabicyclo[4.1.0]heptane-4-carboxylate

Inchi:	InChI=1S/C14H20O4/c15-14(9-2-4-11-13(6-9)18-11)16-7-8-1-3-10-12(5-8)17-10/h8-13H,1
InchiKey:	YXALYBMHAYZKAP-UHFFFAOYSA-N
Formula:	C14H20O4
SMILES:	<chem>O=C(OCC1CCC2OC2C1)C1CCC2OC2C1</chem>
Mol. weight [g/mol]:	252.31
CAS:	2386-87-0

Physical Properties

Property code	Value	Unit	Source
hfus	42.82	kJ/mol	Joback Method
logp	1.665		Crippen Method
mcvol	183.860	ml/mol	McGowan Method
tb	617.88	K	Cheméo Relay (1.0)
tf	236.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

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	-1.49119e+02
Coeff. B	1.80440e+00
Coeff. C	-1.29260e-03
Coeff. D	3.61900e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
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Property code	dvisc
Equation	$Y = \exp(A + B/T + C \cdot \ln(T) + D \cdot T^E)$
Y unit	Pa·s
Coeff. A	-6.02434e+00
Coeff. B	3.40140e+02
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.	236.15
Temperature range (K), max.	616.13

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

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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