m-Cumenyl methylcarbamate

Inchi: InChI=1S/C11H15NO2/c1-8(2)9-5-4-6-10(7-9)14-11(13)12-3/h4-8H,1-3H3,(H,12,13)
InchiKey: GYKXQTKSWLAUIT-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CNC(=O)Oc1cccc(C(C)C)c1
Mol. weight [g/mol]: 193.25
CAS: 64-00-6

Physical Properties

Property code	Value	Unit	Source
af	0.6225		Cheméo Relay (1.0)
hf	-367.03	kJ/mol	Cheméo Relay (1.0)
hfus	23.84	kJ/mol	Joback Method
hvap	81.72	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.27		Cheméo Relay (1.0)
logp	2.528		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
tb	531.53	K	Cheméo Relay (1.0)
tc	777.98	K	Cheméo Relay (1.0)
tf	346.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	0.568	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	-4.20000e+00
Coeff. B	9.37760e-01
Coeff. C	-4.95960e-04
Coeff. D	7.32000e-08

Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

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):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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

Latest version available from:
https://www.chemeo.com/cid/109-646-4/m-Cumenyl-methylcarbamate.pdf
Generated by Cheméo on 2026-10-31 06:00:53.345339692 +0000 UTC m=+50166.272176969.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.