

2-(2-prop-2-enoxycarbonyloxyethoxy)ethyl prop-2-enyl carbonate

Inchi: InChI=1S/C12H18O7/c1-3-5-16-11(13)18-9-7-15-8-10-19-12(14)17-6-4-2/h3-4H,1-2,5-10
InchiKey: JHQVCQDWGSXTFE-UHFFFAOYSA-N
Formula: C12H18O7
SMILES: C=CCOC(=O)OCCOCCOC(=O)OCC=C
Mol. weight [g/mol]: 274.27
CAS: 142-22-3

Physical Properties

Property code	Value	Unit	Source
hf	-1151.28	kJ/mol	Cheméo Relay (1.0)
hfus	36.58	kJ/mol	Joback Method
hvap	88.71	kJ/mol	Cheméo Relay (1.0)
ie	9.71	eV	Cheméo Relay (1.0)
logp	1.681		Crippen Method
mcvol	203.830	ml/mol	McGowan Method
tb	598.25	K	Cheméo Relay (1.0)
tc	707.24	K	Cheméo Relay (1.0)
tf	269.15	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	1.13316e+02
Coeff. B	8.04600e-01
Coeff. C	-1.52600e-04
Coeff. D	-1.12200e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00

Temperature range (K), max.	1000.00
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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	-1.34339e+01
Coeff. B	2.45575e+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.	269.15
Temperature range (K), max.	579.60

Sources

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

Cheméo Relay (1.0):

Legend

cp_g:	Ideal gas heat capacity
dv_{isc}:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hf_{us}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point

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