Docosyl ethyl carbonate

Inchi: InChI=1S/C25H50O3/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-28
InchiKey: XNOOMPASPXIFLV-UHFFFAOYSA-N
Formula: C25H50O3
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCOC(=O)OCC
Mol. weight [g/mol]: 398.66

Physical Properties

Property code	Value	Unit	Source
gf	-179.30	kJ/mol	Joback Method
hf	-936.35	kJ/mol	Joback Method
hfus	64.48	kJ/mol	Joback Method
hvap	82.81	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	8.981		Crippen Method
mcvol	376.420	ml/mol	McGowan Method
pc	776.34	kPa	Joback Method
rinpol	2775.00		NIST Webbook
rinpol	2775.00		NIST Webbook
tb	870.11	K	Joback Method
tc	1066.69	K	Joback Method
tf	465.90	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1255.08	J/mol×K	870.11	Joback Method
cpg	1277.28	J/mol×K	902.87	Joback Method
cpg	1298.10	J/mol×K	935.64	Joback Method
cpg	1317.57	J/mol×K	968.40	Joback Method
cpg	1335.75	J/mol×K	1001.16	Joback Method
cpg	1352.65	J/mol×K	1033.93	Joback Method
cpg	1368.31	J/mol×K	1066.69	Joback Method
dvisc	0.0006233	Pa×s	465.90	Joback Method

dvisc	0.0002650	Pa×s	533.27	Joback Method
dvisc	0.0001365	Pa×s	600.64	Joback Method
dvisc	0.0000803	Pa×s	668.00	Joback Method
dvisc	0.0000521	Pa×s	735.37	Joback Method
dvisc	0.0000364	Pa×s	802.74	Joback Method
dvisc	0.0000268	Pa×s	870.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373792&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume