

Allyl heneicosanoate

Inchi:	InChI=1S/C24H46O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24(25)26
InchiKey:	VMAYYPRDLBOBIR-UHFFFAOYSA-N
Formula:	C24H46O2
SMILES:	C=CCOC(=O)CCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	366.62

Physical Properties

Property code	Value	Unit	Source
gf	5.12	kJ/mol	Joback Method
hf	-658.06	kJ/mol	Joback Method
hfus	59.42	kJ/mol	Joback Method
hvap	77.50	kJ/mol	Joback Method
log10ws	-8.58		Crippen Method
logp	8.147		Crippen Method
mcvol	352.160	ml/mol	McGowan Method
pc	848.01	kPa	Joback Method
rinpol	2549.00		NIST Webbook
rinpol	2549.00		NIST Webbook
tb	821.49	K	Joback Method
tc	1005.89	K	Joback Method
tf	430.64	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.16	J/molxK	821.49	Joback Method
cpg	1150.21	J/molxK	852.22	Joback Method
cpg	1170.15	J/molxK	882.96	Joback Method
cpg	1189.00	J/molxK	913.69	Joback Method
cpg	1206.82	J/molxK	944.43	Joback Method
cpg	1223.63	J/molxK	975.16	Joback Method
cpg	1239.49	J/molxK	1005.89	Joback Method
dvisc	0.0010688	Paxs	430.64	Joback Method

dvisc	0.0004448	Paxs	495.78	Joback Method
dvisc	0.0002269	Paxs	560.92	Joback Method
dvisc	0.0001332	Paxs	626.07	Joback Method
dvisc	0.0000864	Paxs	691.21	Joback Method
dvisc	0.0000604	Paxs	756.35	Joback Method
dvisc	0.0000447	Paxs	821.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541121&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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