

Allyl heptadecanoate

Inchi: InChI=1S/C20H38O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20(21)22-19-4-2/h4H,1
InchiKey: XDMYOMNKAQFDX-UHFFFAOYSA-N
Formula: C20H38O2
SMILES: C=CCOC(=O)CCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 310.51

Physical Properties

Property code	Value	Unit	Source
gf	-28.56	kJ/mol	Joback Method
hf	-575.50	kJ/mol	Joback Method
hfus	49.06	kJ/mol	Joback Method
hvap	68.60	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	6.587		Crippen Method
mvol	295.800	ml/mol	McGowan Method
pc	1074.98	kPa	Joback Method
rinpol	2152.00		NIST Webbook
rinpol	2152.00		NIST Webbook
tb	729.97	K	Joback Method
tc	902.05	K	Joback Method
tf	385.56	K	Joback Method
vc	1.161	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.13	J/molxK	729.97	Joback Method
cpg	970.07	J/molxK	873.37	Joback Method
cpg	954.38	J/molxK	844.69	Joback Method
cpg	937.86	J/molxK	816.01	Joback Method
cpg	920.50	J/molxK	787.33	Joback Method
cpg	902.27	J/molxK	758.65	Joback Method
cpg	984.96	J/molxK	902.05	Joback Method
dvisc	0.0000776	Paxs	729.97	Joback Method

dvisc	0.0001040	Paxs	672.57	Joback Method
dvisc	0.0001470	Paxs	615.17	Joback Method
dvisc	0.0002232	Paxs	557.76	Joback Method
dvisc	0.0003730	Paxs	500.36	Joback Method
dvisc	0.0007121	Paxs	442.96	Joback Method
dvisc	0.0016482	Paxs	385.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541136&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
hvap:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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