allyl palmitate

Inchi: InChI=1S/C19H36O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-19(20)21-18-4-2/h4H,2-3,
InchiKey: HAFZJTKIBGEQKT-UHFFFAOYSA-N
Formula: C19H36O2
SMILES: C=CCOC(=O)CCCCCCCCCCCCCCC
Mol. weight [g/mol]: 296.49
CAS: 43211-62-7

Physical Properties

Property code	Value	Unit	Source
af	0.8964		Cheméo Relay (1.0)
gf	-36.98	kJ/mol	Joback Method
hf	-641.99	kJ/mol	Cheméo Relay (1.0)
hfus	46.47	kJ/mol	Joback Method
hvap	93.57	kJ/mol	Cheméo Relay (1.0)
ie	9.70	eV	Cheméo Relay (1.0)
log10ws	-6.44		Cheméo Relay (1.0)
logp	6.197		Crippen Method
mcvol	281.710	ml/mol	McGowan Method
pc	1145.99	kPa	Joback Method
tb	604.41	K	Cheméo Relay (1.0)
tc	773.08	K	Cheméo Relay (1.0)
tf	281.20	K	Cheméo Relay (1.0)
vc	1.070	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.93	J/mol×K	707.09	Joback Method
cpg	923.77	J/mol×K	877.73	Joback Method
cpg	909.12	J/mol×K	849.29	Joback Method
cpg	893.71	J/mol×K	820.85	Joback Method
cpg	877.51	J/mol×K	792.41	Joback Method
cpg	860.49	J/mol×K	763.97	Joback Method
cpg	842.64	J/mol×K	735.53	Joback Method

dvisc	0.0002517	Pa×s	540.69	Joback Method
dvisc	0.0000884	Pa×s	707.09	Joback Method
dvisc	0.0001181	Pa×s	651.62	Joback Method
dvisc	0.0001664	Pa×s	596.16	Joback Method
dvisc	0.0018146	Pa×s	374.29	Joback Method
dvisc	0.0004182	Pa×s	485.22	Joback Method
dvisc	0.0007925	Pa×s	429.76	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C43211627&Units=SI

Joback Method: 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

af: Acentric Factor
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
ie: Ionization energy
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: