

Eugenyl hexanoate

Inchi:	InChI=1S/C16H22O3/c1-4-6-7-9-16(17)19-14-11-10-13(8-5-2)12-15(14)18-3/h5,10-12H,2
InchiKey:	CBTUXJRFSPCNEZ-UHFFFAOYSA-N
Formula:	C16H22O3
SMILES:	<chem>C=CCc1ccc(OC(=O)CCCC)c(OC)c1</chem>
Mol. weight [g/mol]:	262.34

Physical Properties

Property code	Value	Unit	Source
gf	-74.09	kJ/mol	Joback Method
hf	-411.57	kJ/mol	Joback Method
hfus	33.15	kJ/mol	Joback Method
hvap	65.71	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.909		Crippen Method
mvol	221.550	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	1917.00		NIST Webbook
rinpol	1917.00		NIST Webbook
tb	697.51	K	Joback Method
tc	896.32	K	Joback Method
tf	414.17	K	Joback Method
vc	0.847	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.95	J/molxK	697.51	Joback Method
cpg	675.05	J/molxK	863.18	Joback Method
cpg	662.58	J/molxK	830.05	Joback Method
cpg	649.24	J/molxK	796.91	Joback Method
cpg	635.04	J/molxK	763.78	Joback Method
cpg	619.94	J/molxK	730.64	Joback Method
cpg	686.67	J/molxK	896.32	Joback Method
dvisc	0.0000988	Paxs	697.51	Joback Method

dvisc	0.0001238	Paxs	650.29	Joback Method
dvisc	0.0001609	Paxs	603.06	Joback Method
dvisc	0.0002185	Paxs	555.84	Joback Method
dvisc	0.0003141	Paxs	508.62	Joback Method
dvisc	0.0004864	Paxs	461.39	Joback Method
dvisc	0.0008322	Paxs	414.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224910&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
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	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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