

Vanillic acid, heptyl ester

Inchi:	InChI=1S/C15H22O4/c1-3-4-5-6-7-10-19-15(17)12-8-9-13(16)14(11-12)18-2/h8-9,11,16H
InchiKey:	DAJVWKLZJELSB-UHFFFAOYSA-N
Formula:	C15H22O4
SMILES:	CCCCCCCOC(=O)c1ccc(O)c(OC)c1
Mol. weight [g/mol]:	266.33
CAS:	84375-72-4

Physical Properties

Property code	Value	Unit	Source
gf	-315.34	kJ/mol	Joback Method
hf	-682.20	kJ/mol	Joback Method
hfus	38.02	kJ/mol	Joback Method
hvap	76.50	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.528		Crippen Method
mcvol	217.630	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
tb	753.59	K	Joback Method
tc	959.75	K	Joback Method
tf	503.86	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.31	J/molxK	753.59	Joback Method
cpg	645.94	J/molxK	787.95	Joback Method
cpg	659.76	J/molxK	822.31	Joback Method
cpg	672.81	J/molxK	856.67	Joback Method
cpg	685.16	J/molxK	891.03	Joback Method
cpg	696.83	J/molxK	925.39	Joback Method
cpg	707.87	J/molxK	959.75	Joback Method
dvisc	0.0001648	Paxs	503.86	Joback Method
dvisc	0.0000808	Paxs	545.48	Joback Method

dvisc	0.0000438	Paxs	587.10	Joback Method
dvisc	0.0000258	Paxs	628.73	Joback Method
dvisc	0.0000162	Paxs	670.35	Joback Method
dvisc	0.0000107	Paxs	711.97	Joback Method
dvisc	0.0000074	Paxs	753.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84375724&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/12-969-3/Vanillic-acid-heptyl-ester.pdf>

Generated by Cheméo on 2024-04-26 09:53:33.774476265 +0000 UTC m=+16414462.695053577.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.