

Glycolic acid, phenethyl ester

Inchi:	InChI=1S/C10H12O3/c11-8-10(12)13-7-6-9-4-2-1-3-5-9/h1-5,11H,6-8H2
InchiKey:	GCWBOYJHPSTLAU-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	O=C(CO)OCCc1ccccc1
Mol. weight [g/mol]:	180.20
CAS:	72928-38-2

Physical Properties

Property code	Value	Unit	Source
gf	-225.01	kJ/mol	Joback Method
hf	-410.23	kJ/mol	Joback Method
hfus	22.57	kJ/mol	Joback Method
hvap	65.97	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	0.765		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
tb	623.35	K	Joback Method
tc	821.89	K	Joback Method
tf	361.86	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.28	J/molxK	623.35	Joback Method
cpg	400.65	J/molxK	788.80	Joback Method
cpg	392.00	J/molxK	755.71	Joback Method
cpg	382.76	J/molxK	722.62	Joback Method
cpg	372.90	J/molxK	689.53	Joback Method
cpg	362.42	J/molxK	656.44	Joback Method
cpg	408.71	J/molxK	821.89	Joback Method
dvisc	0.0000688	Paxs	623.35	Joback Method
dvisc	0.0001033	Paxs	579.77	Joback Method

dvisc	0.0001658	Paxs	536.19	Joback Method
dvisc	0.0002893	Paxs	492.61	Joback Method
dvisc	0.0005624	Paxs	449.02	Joback Method
dvisc	0.0012611	Paxs	405.44	Joback Method
dvisc	0.0034351	Paxs	361.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72928382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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/40-088-0/Glycolic-acid-phenethyl-ester.pdf>

Generated by Cheméo on 2024-04-23 16:41:00.711705715 +0000 UTC m=+16179709.632283026.

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