

Glyceryl p-coumarate

Inchi:	InChI=1S/C12H14O5/c13-7-11(15)8-17-12(16)6-3-9-1-4-10(14)5-2-9/h1-6,11,13-15H,7-8
InchiKey:	YUQSZTOOHLGKGG-ZZXKVVIFSA-N
Formula:	C12H14O5
SMILES:	O=C(C=Cc1ccc(O)cc1)OCC(O)CO
Mol. weight [g/mol]:	238.24
CAS:	106055-11-2

Physical Properties

Property code	Value	Unit	Source
gf	-421.83	kJ/mol	Joback Method
hf	-669.11	kJ/mol	Joback Method
hfus	34.30	kJ/mol	Joback Method
hvap	99.68	kJ/mol	Joback Method
log10ws	-1.02		Crippen Method
logp	0.302		Crippen Method
mcvol	176.930	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
rinpol	2430.50		NIST Webbook
rinpol	2430.50		NIST Webbook
tb	845.63	K	Joback Method
tc	1052.06	K	Joback Method
tf	536.86	K	Joback Method
vc	0.602	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.99	J/mol×K	845.63	Joback Method
cpg	528.05	J/mol×K	880.03	Joback Method
cpg	536.73	J/mol×K	914.44	Joback Method
cpg	545.11	J/mol×K	948.84	Joback Method
cpg	553.24	J/mol×K	983.25	Joback Method
cpg	561.20	J/mol×K	1017.65	Joback Method
cpg	569.07	J/mol×K	1052.06	Joback Method

dvisc	0.0000442	Paxs	536.86	Joback Method
dvisc	0.0000124	Paxs	588.32	Joback Method
dvisc	0.0000043	Paxs	639.78	Joback Method
dvisc	0.0000017	Paxs	691.25	Joback Method
dvisc	0.0000008	Paxs	742.71	Joback Method
dvisc	0.0000004	Paxs	794.17	Joback Method
dvisc	0.0000002	Paxs	845.63	Joback Method

Sources

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=C106055112&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
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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