

Fumaric acid, propyl tetradec-3-enyl ester

Inchi: InChI=1S/C21H36O4/c1-3-5-6-7-8-9-10-11-12-13-14-15-19-25-21(23)17-16-20(22)24-18
InchiKey: GMIULCVRRHFMOX-VLDVYECUSA-N
Formula: C21H36O4
SMILES: CCCCCCCCCC=CCCOC(=O)C=CC(=O)OCCC
Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-181.46	kJ/mol	Joback Method
hf	-731.93	kJ/mol	Joback Method
hfus	56.12	kJ/mol	Joback Method
hvap	80.57	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.516		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1083.49	kPa	Joback Method
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook
tb	840.78	K	Joback Method
tc	1032.19	K	Joback Method
tf	460.59	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.48	J/molxK	840.78	Joback Method
cpg	1056.73	J/molxK	1000.29	Joback Method
cpg	1042.91	J/molxK	968.39	Joback Method
cpg	1028.21	J/molxK	936.48	Joback Method
cpg	1012.60	J/molxK	904.58	Joback Method
cpg	996.04	J/molxK	872.68	Joback Method
cpg	1069.73	J/molxK	1032.19	Joback Method
dvisc	0.0000350	Paxs	840.78	Joback Method

dvisc	0.0000467	Paxs	777.42	Joback Method
dvisc	0.0000655	Paxs	714.05	Joback Method
dvisc	0.0000984	Paxs	650.69	Joback Method
dvisc	0.0001611	Paxs	587.32	Joback Method
dvisc	0.0002974	Paxs	523.96	Joback Method
dvisc	0.0006498	Paxs	460.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348120&Units=SI

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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