

Fumaric acid, 3-heptyl propyl ester

Inchi:	InChI=1S/C14H24O4/c1-4-7-8-12(6-3)18-14(16)10-9-13(15)17-11-5-2/h9-10,12H,4-8,11H
InchiKey:	WRPCOPQOIPNZGI-MDZDMXLPSA-N
Formula:	C14H24O4
SMILES:	CCCCC(CC)OC(=O)C=CC(=O)OCCC
Mol. weight [g/mol]:	256.34

Physical Properties

Property code	Value	Unit	Source
gf	-323.06	kJ/mol	Joback Method
hf	-709.95	kJ/mol	Joback Method
hfus	34.27	kJ/mol	Joback Method
hvap	64.64	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.008		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
rinpol	1685.00		NIST Webbook
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tb	676.02	K	Joback Method
tc	859.88	K	Joback Method
tf	371.78	K	Joback Method
vc	0.842	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.60	J/molxK	676.02	Joback Method
cpg	616.00	J/molxK	706.66	Joback Method
cpg	630.64	J/molxK	737.31	Joback Method
cpg	644.52	J/molxK	767.95	Joback Method
cpg	657.67	J/molxK	798.59	Joback Method
cpg	670.09	J/molxK	829.24	Joback Method
cpg	681.79	J/molxK	859.88	Joback Method
dvisc	0.0017024	Paxs	371.78	Joback Method

dvisc	0.0007897	Paxs	422.49	Joback Method
dvisc	0.0004319	Paxs	473.19	Joback Method
dvisc	0.0002655	Paxs	523.90	Joback Method
dvisc	0.0001778	Paxs	574.61	Joback Method
dvisc	0.0001271	Paxs	625.31	Joback Method
dvisc	0.0000955	Paxs	676.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348678&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
mccvol:	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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