

Adipic acid, pent-4-enyl propyl ester

Inchi:	InChI=1S/C14H24O4/c1-3-5-8-12-18-14(16)10-7-6-9-13(15)17-11-4-2/h3H,1,4-12H2,2H3
InchiKey:	XAJGWDCLNPIWMB-UHFFFAOYSA-N
Formula:	C14H24O4
SMILES:	C=CCCCOC(=O)CCCC(=O)OCCC
Mol. weight [g/mol]:	256.34

Physical Properties

Property code	Value	Unit	Source
gf	-313.00	kJ/mol	Joback Method
hf	-696.46	kJ/mol	Joback Method
hfus	36.31	kJ/mol	Joback Method
hvap	64.40	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.009		Crippen Method
mvol	218.700	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
rinpol	1757.00		NIST Webbook
rinpol	1757.00		NIST Webbook
tb	668.98	K	Joback Method
tc	847.08	K	Joback Method
tf	390.10	K	Joback Method
vc	0.849	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.95	J/molxK	668.98	Joback Method
cpg	614.06	J/molxK	698.66	Joback Method
cpg	628.45	J/molxK	728.35	Joback Method
cpg	642.14	J/molxK	758.03	Joback Method
cpg	655.12	J/molxK	787.71	Joback Method
cpg	667.41	J/molxK	817.40	Joback Method
cpg	679.01	J/molxK	847.08	Joback Method
dvisc	0.0014702	Paxs	390.10	Joback Method

dvisc	0.0007848	Paxs	436.58	Joback Method
dvisc	0.0004727	Paxs	483.06	Joback Method
dvisc	0.0003112	Paxs	529.54	Joback Method
dvisc	0.0002192	Paxs	576.02	Joback Method
dvisc	0.0001627	Paxs	622.50	Joback Method
dvisc	0.0001259	Paxs	668.98	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=U353791&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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