

Adipic acid, ethyl trans-hex-3-enyl ester

Inchi:	InChI=1S/C14H24O4/c1-3-5-6-9-12-18-14(16)11-8-7-10-13(15)17-4-2/h5-6H,3-4,7-12H2
InchiKey:	FGZYSRAQEERBII-AATRIKPKSA-N
Formula:	C14H24O4
SMILES:	CCC=CCCOC(=O)CCCCC(=O)OCC
Mol. weight [g/mol]:	256.34

Physical Properties

Property code	Value	Unit	Source
gf	-320.62	kJ/mol	Joback Method
hf	-704.67	kJ/mol	Joback Method
hfus	37.79	kJ/mol	Joback Method
hvap	65.03	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.009		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	1762.00		NIST Webbook
rinpol	1762.00		NIST Webbook
tb	676.46	K	Joback Method
tc	857.71	K	Joback Method
tf	386.78	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.12	J/mol×K	676.46	Joback Method
cpg	668.66	J/mol×K	827.50	Joback Method
cpg	656.37	J/mol×K	797.29	Joback Method
cpg	643.39	J/mol×K	767.08	Joback Method
cpg	629.69	J/mol×K	736.88	Joback Method
cpg	615.28	J/mol×K	706.67	Joback Method
cpg	680.26	J/mol×K	857.71	Joback Method
dvisc	0.0001031	Pa×s	676.46	Joback Method

dvisc	0.0001345	Pa×s	628.18	Joback Method
dvisc	0.0001834	Pa×s	579.90	Joback Method
dvisc	0.0002647	Pa×s	531.62	Joback Method
dvisc	0.0004109	Pa×s	483.34	Joback Method
dvisc	0.0007034	Pa×s	435.06	Joback Method
dvisc	0.0013772	Pa×s	386.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U354005&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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