

Adipic acid, cis-hex-3-enyl ethyl 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-WAYWQWQTS-A-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
mvol	218.700	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	676.46	K	Joback Method
tc	857.71	K	Joback Method
tf	386.78	K	Joback Method
vc	0.848	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.12	J/mol×K	676.46	Joback Method
cpg	615.28	J/mol×K	706.67	Joback Method
cpg	629.69	J/mol×K	736.88	Joback Method
cpg	643.39	J/mol×K	767.08	Joback Method
cpg	656.37	J/mol×K	797.29	Joback Method
cpg	668.66	J/mol×K	827.50	Joback Method
cpg	680.26	J/mol×K	857.71	Joback Method
dvisc	0.0013772	Paxs	386.78	Joback Method

dvisc	0.0007034	Paxs	435.06	Joback Method
dvisc	0.0004109	Paxs	483.34	Joback Method
dvisc	0.0002647	Paxs	531.62	Joback Method
dvisc	0.0001834	Paxs	579.90	Joback Method
dvisc	0.0001345	Paxs	628.18	Joback Method
dvisc	0.0001031	Paxs	676.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353969&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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