

Adipic acid, di(pent-4-enyl) ester

Inchi: InChI=1S/C16H26O4/c1-3-5-9-13-19-15(17)11-7-8-12-16(18)20-14-10-6-4-2/h3-4H,1-2,5H
InchiKey: ATARNRXKSIAJEH-UHFFFAOYSA-N
Formula: C16H26O4
SMILES: C=CCCCOC(=O)CCCCC(=O)OCCCC=C
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-208.32	kJ/mol	Joback Method
hf	-612.31	kJ/mol	Joback Method
hfus	40.21	kJ/mol	Joback Method
hvap	68.18	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.566		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1504.65	kPa	Joback Method
rinpol	1948.00		NIST Webbook
rinpol	1948.00		NIST Webbook
tb	711.42	K	Joback Method
tc	891.01	K	Joback Method
tf	410.88	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.63	J/mol×K	711.42	Joback Method
cpg	754.46	J/mol×K	861.07	Joback Method
cpg	742.02	J/mol×K	831.14	Joback Method
cpg	728.83	J/mol×K	801.21	Joback Method
cpg	714.87	J/mol×K	771.28	Joback Method
cpg	700.15	J/mol×K	741.35	Joback Method
cpg	766.16	J/mol×K	891.01	Joback Method
dvisc	0.0001034	Pa×s	711.42	Joback Method

dvisc	0.0001339	Pa×s	661.33	Joback Method
dvisc	0.0001808	Pa×s	611.24	Joback Method
dvisc	0.0002575	Pa×s	561.15	Joback Method
dvisc	0.0003932	Pa×s	511.06	Joback Method
dvisc	0.0006583	Pa×s	460.97	Joback Method
dvisc	0.0012494	Pa×s	410.88	Joback Method

Sources

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=U353809&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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