

Adipic acid, heptadecyl pent-4-enyl ester

Inchi:	InChI=1S/C28H52O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-22-26-32-28(30)24-20-1
InchiKey:	ZWERQCUOKMSVFF-UHFFFAOYSA-N
Formula:	C28H52O4
SMILES:	C=CCCCOC(=O)CCCC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	452.71

Physical Properties

Property code	Value	Unit	Source
gf	-195.12	kJ/mol	Joback Method
hf	-985.42	kJ/mol	Joback Method
hfus	72.57	kJ/mol	Joback Method
hvap	95.56	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.471		Crippen Method
mcvol	415.960	ml/mol	McGowan Method
pc	702.84	kPa	Joback Method
rinpol	3127.00		NIST Webbook
tb	989.30	K	Joback Method
tc	1226.22	K	Joback Method
tf	547.88	K	Joback Method
vc	1.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1444.22	J/molxK	989.30	Joback Method
cpg	1466.32	J/molxK	1028.79	Joback Method
cpg	1486.51	J/molxK	1068.27	Joback Method
cpg	1504.89	J/molxK	1107.76	Joback Method
cpg	1521.51	J/molxK	1147.25	Joback Method
cpg	1536.48	J/molxK	1186.74	Joback Method
cpg	1549.85	J/molxK	1226.22	Joback Method
dvisc	0.0003251	Paxs	547.88	Joback Method
dvisc	0.0001487	Paxs	621.45	Joback Method

dvisc	0.0000803	Paxs	695.02	Joback Method
dvisc	0.0000488	Paxs	768.59	Joback Method
dvisc	0.0000323	Paxs	842.16	Joback Method
dvisc	0.0000229	Paxs	915.73	Joback Method
dvisc	0.0000171	Paxs	989.30	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=U353806&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
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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