

Adipic acid, pent-4-enyl tetradecyl ester

Inchi: InChI=1S/C25H46O4/c1-3-5-7-8-9-10-11-12-13-14-15-19-23-29-25(27)21-17-16-20-24(28)
InchiKey: LKBZUKWYUUKCKP-UHFFFAOYSA-N
Formula: C25H46O4
SMILES: C=CCCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	-220.38	kJ/mol	Joback Method
hf	-923.50	kJ/mol	Joback Method
hfus	64.80	kJ/mol	Joback Method
hvap	88.89	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	7.300		Crippen Method
mvol	373.690	ml/mol	McGowan Method
pc	823.84	kPa	Joback Method
rinpol	2817.00		NIST Webbook
rinpol	2817.00		NIST Webbook
tb	920.66	K	Joback Method
tc	1129.75	K	Joback Method
tf	514.07	K	Joback Method
vc	1.464	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1251.87	J/molxK	920.66	Joback Method
cpg	1272.01	J/molxK	955.51	Joback Method
cpg	1290.71	J/molxK	990.36	Joback Method
cpg	1308.00	J/molxK	1025.21	Joback Method
cpg	1323.94	J/molxK	1060.05	Joback Method
cpg	1338.57	J/molxK	1094.90	Joback Method
cpg	1351.93	J/molxK	1129.75	Joback Method
dvisc	0.0004774	Paxs	514.07	Joback Method

dvisc	0.0002242	Paxs	581.84	Joback Method
dvisc	0.0001233	Paxs	649.60	Joback Method
dvisc	0.0000759	Paxs	717.37	Joback Method
dvisc	0.0000508	Paxs	785.13	Joback Method
dvisc	0.0000362	Paxs	852.89	Joback Method
dvisc	0.0000272	Paxs	920.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353803&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.cheméo.com/cid/49-153-8/Adipic-acid-pent-4-enyl-tetradecyl-ester.pdf>

Generated by Cheméo on 2024-04-26 15:28:20.383161865 +0000 UTC m=+16434549.303739187.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.