

Adipic acid, 2,4-dimethylpent-3-yl tridecyl ester

Inchi:	InChI=1S/C26H50O4/c1-6-7-8-9-10-11-12-13-14-15-18-21-29-24(27)19-16-17-20-25(28)
InchiKey:	GLMIQPJONLFJGB-UHFFFAOYSA-N
Formula:	C26H50O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	426.67

Physical Properties

Property code	Value	Unit	Source
gf	-307.12	kJ/mol	Joback Method
hf	-1085.41	kJ/mol	Joback Method
hfus	58.10	kJ/mol	Joback Method
hvap	90.62	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	7.625		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	772.46	kPa	Joback Method
rinsol	2780.00		NIST Webbook
tb	945.54	K	Joback Method
tc	1161.05	K	Joback Method
tf	482.10	K	Joback Method
vc	1.522	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1346.32	J/molxK	945.54	Joback Method
cpg	1367.21	J/molxK	981.46	Joback Method
cpg	1386.45	J/molxK	1017.38	Joback Method
cpg	1404.07	J/molxK	1053.29	Joback Method
cpg	1420.12	J/molxK	1089.21	Joback Method
cpg	1434.66	J/molxK	1125.13	Joback Method
cpg	1447.72	J/molxK	1161.05	Joback Method
dvisc	0.0006421	Paxs	482.10	Joback Method
dvisc	0.0002284	Paxs	559.34	Joback Method

dvisc	0.0001044	Paxs	636.58	Joback Method
dvisc	0.0000565	Paxs	713.82	Joback Method
dvisc	0.0000345	Paxs	791.06	Joback Method
dvisc	0.0000230	Paxs	868.30	Joback Method
dvisc	0.0000164	Paxs	945.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353530&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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.chemeo.com/cid/20-403-1/Adipic-acid-2-4-dimethylpent-3-yl-tridecyl-ester.pdf>

Generated by Cheméo on 2024-04-25 18:00:15.54739703 +0000 UTC m=+16357264.467974343.

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