Adipic acid, 2,3-dimethylphenyl undecyl ester

Inchi: InChI=1S/C25H40O4/c1-4-5-6-7-8-9-10-11-14-20-28-24(26)18-12-13-19-25(27)29-23-17
InchiKey: SCIRNMPNTLEGLT-UHFFFAOYSA-N
Formula: C25H40O4
SMILES: CCCCCCCCCCCOC(=O)CCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 404.58

Physical Properties

Property code	Value	Unit	Source
gf	-215.07	kJ/mol	Joback Method
hf	-835.34	kJ/mol	Joback Method
hfus	59.34	kJ/mol	Joback Method
hvap	93.16	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	6.843		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	961.48	kPa	Joback Method
rinpol	2989.00		NIST Webbook
tb	960.62	K	Joback Method
tc	1176.07	K	Joback Method
tf	567.29	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.77	J/mol×K	960.62	Joback Method
cpg	1252.28	J/mol×K	1140.16	Joback Method
cpg	1240.78	J/mol×K	1104.25	Joback Method
cpg	1227.92	J/mol×K	1068.35	Joback Method
cpg	1213.65	J/mol×K	1032.44	Joback Method
cpg	1197.95	J/mol×K	996.53	Joback Method
cpg	1262.45	J/mol×K	1176.07	Joback Method
dvisc	0.0000271	Pa×s	960.62	Joback Method
dvisc	0.0000349	Pa×s	895.06	Joback Method

dvisc	0.0000469	Pa×s	829.51	Joback Method
dvisc	0.0000662	Pa×s	763.95	Joback Method
dvisc	0.0000997	Pa×s	698.40	Joback Method
dvisc	0.0001634	Pa×s	632.84	Joback Method
dvisc	0.0003003	Pa×s	567.29	Joback Method

Sources

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=U353888&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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