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

Inchi: InChI=1S/C25H48O4/c1-6-7-8-9-10-11-12-13-14-17-20-28-23(26)18-15-16-19-24(27)29-

InchiKey: XKNSKFDIWOSAJT-UHFFFAOYSA-N

Formula: C25H48O4

SMILES: CCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
gf	-315.54	kJ/mol	Joback Method
hf	-1064.77	kJ/mol	Joback Method
hfus	55.51	kJ/mol	Joback Method
hvap	88.39	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	7.235		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	815.39	kPa	Joback Method
rinpol	2691.00		NIST Webbook
rinpol	2691.00		NIST Webbook
tb	922.66	K	Joback Method
tc	1130.87	K	Joback Method
tf	470.83	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.35	J/mol×K	922.66	Joback Method
cpg	1302.76	J/mol×K	957.36	Joback Method
cpg	1321.65	J/mol×K	992.06	Joback Method
cpg	1339.04	J/mol×K	1026.76	Joback Method
cpg	1354.98	J/mol×K	1061.46	Joback Method
cpg	1369.52	J/mol×K	1096.16	Joback Method
cpg	1382.68	J/mol×K	1130.87	Joback Method
dvisc	0.0007421	Pa×s	470.83	Joback Method

dvisc	0.0002651	Pa×s	546.13	Joback Method
dvisc	0.0001216	Pa×s	621.44	Joback Method
dvisc	0.0000660	Pa×s	696.75	Joback Method
dvisc	0.0000403	Pa×s	772.05	Joback Method
dvisc	0.0000269	Pa×s	847.36	Joback Method
dvisc	0.0000192	Pa×s	922.66	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U353529&Units=SI

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