(2E,6E)-3,7,11-Trimethyldodeca-2,6,10-trien-1-yl dodecanoate

Inchi: InChI=1S/C27H48O2/c1-6-7-8-9-10-11-12-13-14-21-27(28)29-23-22-26(5)20-16-19-25(4
InchiKey: APTQJZOTWYEACL-HWHBRYGOSA-N
Formula: C27H48O2
SMILES: CCCCCCCCCCCC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 404.67
CAS: 78368-58-8

Physical Properties

Property code	Value	Unit	Source
gf	157.55	kJ/mol	Joback Method
hf	-523.12	kJ/mol	Joback Method
hfus	65.15	kJ/mol	Joback Method
hvap	84.97	kJ/mol	Joback Method
log10ws	-9.55		Crippen Method
logp	8.870		Crippen Method
mcvol	385.830	ml/mol	McGowan Method
pc	774.61	kPa	Joback Method
rinpol	2804.70		NIST Webbook
rinpol	2804.70		NIST Webbook
tb	905.57	K	Joback Method
tc	1108.67	K	Joback Method
tf	409.09	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1269.42	J/mol×K	905.57	Joback Method
cpg	1291.08	J/mol×K	939.42	Joback Method
cpg	1311.67	J/mol×K	973.27	Joback Method
cpg	1331.30	J/mol×K	1007.12	Joback Method
cpg	1350.04	J/mol×K	1040.97	Joback Method
cpg	1368.00	J/mol×K	1074.82	Joback Method
cpg	1385.26	J/mol×K	1108.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78368588&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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/86-264-4/2E-6E-3-7-11-Trimethyldodeca-2-6-10-trien-1-yl-dodecanoate.pdf
Generated by Cheméo on 2024-10-12 05:33:22.933592983 +0000 UTC m=+3292065.570562236.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.