(2E,6E)-3,7,11-Trimethyldodeca-2,6,10-trienyl propionate

Inchi: InChI=1S/C18H30O2/c1-6-18(19)20-14-13-17(5)12-8-11-16(4)10-7-9-15(2)3/h9,11,13H,6
InchiKey: XFACLYNWBJYMCK-IUBLYSDUSA-N
Formula: C18H30O2
SMILES: CCC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 278.43
CAS: 104857-55-8

Physical Properties

Property code	Value	Unit	Source
gf	81.77	kJ/mol	Joback Method
hf	-337.36	kJ/mol	Joback Method
hfus	41.84	kJ/mol	Joback Method
hvap	64.93	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.359		Crippen Method
mcvol	259.020	ml/mol	McGowan Method
pc	1342.74	kPa	Joback Method
rinpol	1933.20		NIST Webbook
rinpol	1933.20		NIST Webbook
tb	699.65	K	Joback Method
tc	887.99	K	Joback Method
tf	307.66	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.44	J/mol×K	699.65	Joback Method
cpg	740.39	J/mol×K	731.04	Joback Method
cpg	757.44	J/mol×K	762.43	Joback Method
cpg	773.65	J/mol×K	793.82	Joback Method
cpg	789.07	J/mol×K	825.21	Joback Method
cpg	803.75	J/mol×K	856.60	Joback Method
cpg	817.75	J/mol×K	887.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104857558&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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