(E)-3,7-Dimethylocta-2,6-dien-1-yl icosanoate

Inchi: InChI=1S/C30H56O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-30(31)32-2
InchiKey: BEDGRFXPXOLZFD-PBBVDAKRSA-N
Formula: C30H56O2
SMILES: CCCCCCCCCCCCCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 448.76
CAS: 467252-74-0

Physical Properties

Property code	Value	Unit	Source
gf	111.14	kJ/mol	Joback Method
hf	-692.47	kJ/mol	Joback Method
hfus	74.03	kJ/mol	Joback Method
hvap	91.61	kJ/mol	Joback Method
log10ws	-10.95		Crippen Method
logp	10.264		Crippen Method
mcvol	432.400	ml/mol	McGowan Method
pc	644.83	kPa	Joback Method
rinpol	3156.50		NIST Webbook
rinpol	3156.50		NIST Webbook
tb	970.17	K	Joback Method
tc	1195.95	K	Joback Method
tf	461.94	K	Joback Method
vc	1.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1493.25	J/mol×K	970.17	Joback Method
cpg	1517.85	J/mol×K	1007.80	Joback Method
cpg	1541.03	J/mol×K	1045.43	Joback Method
cpg	1562.91	J/mol×K	1083.06	Joback Method
cpg	1583.62	J/mol×K	1120.69	Joback Method
cpg	1603.27	J/mol×K	1158.32	Joback Method
cpg	1622.00	J/mol×K	1195.95	Joback Method

Sources

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=C467252740&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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