3,7,11-Trimethyl-dodeca-2,6,10-trienoic acid

Other names: (2E,6E)-3,7,11-Trimethyldodeca-2,6,10-trienoic acid
Inchi: InChI=1S/C15H24O2/c1-12(2)7-5-8-13(3)9-6-10-14(4)11-15(16)17/h7,9,11H,5-6,8,10H2,
InchiKey: WJHFZYAELPOJIV-IJFRVEDASA-N
Formula: C15H24O2
SMILES: CC(C)=CCCC(C)=CCCC(C)=CC(=O)O
Mol. weight [g/mol]: 236.35
CAS: 7548-13-2

Physical Properties

Property code	Value	Unit	Source
gf	24.69	kJ/mol	Joback Method
hf	-295.45	kJ/mol	Joback Method
hfus	36.97	kJ/mol	Joback Method
hvap	72.52	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.490		Crippen Method
mcvol	216.750	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	1821.80		NIST Webbook
tb	700.77	K	Joback Method
tc	887.37	K	Joback Method
tf	312.44	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.65	J/mol×K	700.77	Joback Method
cpg	608.92	J/mol×K	731.87	Joback Method
cpg	622.47	J/mol×K	762.97	Joback Method
cpg	635.37	J/mol×K	794.07	Joback Method
cpg	647.67	J/mol×K	825.17	Joback Method
cpg	659.42	J/mol×K	856.27	Joback Method
cpg	670.69	J/mol×K	887.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7548132&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

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