

(Z)-3,7-dimethylocta-2,6-dienyl 2-methylbutyrate

Other names:	(Z)-3,7-Dimethylocta-2,6-dien-1-yl 2-methylbutanoate
Inchi:	InChI=1S/C15H26O2/c1-6-14(5)15(16)17-11-10-13(4)9-7-8-12(2)3/h8,10,14H,6-7,9,11H2
InchiKey:	PEQMAZJTEUEQJP-RAXLEYEMSA-N
Formula:	C15H26O2
SMILES:	CCC(C)C(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	238.37
CAS:	51117-19-2

Physical Properties

Property code	Value	Unit	Source
gf	-17.60	kJ/mol	Joback Method
hf	-388.15	kJ/mol	Joback Method
hfus	31.65	kJ/mol	Joback Method
hvap	57.83	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.268		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	1581.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1571.80		NIST Webbook
tb	626.53	K	Joback Method
tc	813.52	K	Joback Method
tf	277.89	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.04	J/molxK	626.53	Joback Method
cpg	597.38	J/molxK	657.69	Joback Method
cpg	613.87	J/molxK	688.86	Joback Method
cpg	629.53	J/molxK	720.02	Joback Method
cpg	644.42	J/molxK	751.19	Joback Method

cpg	658.56	J/mol×K	782.35	Joback Method
cpg	671.98	J/mol×K	813.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51117192&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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/93-434-7/Z-3-7-dimethylocta-2-6-dienyl-2-methylbutyrate.pdf>

Generated by Cheméo on 2024-04-26 15:45:39.584923814 +0000 UTC m=+16435588.505501136.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.