3,7-Dimethyloct-6-en-1-yl heptanoate

Inchi: InChI=1S/C17H32O2/c1-5-6-7-8-12-17(18)19-14-13-16(4)11-9-10-15(2)3/h10,16H,5-9,11
InchiKey: JZTNHMKNNVAGPD-UHFFFAOYSA-N
Formula: C17H32O2
SMILES: CCCCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 268.44

Physical Properties

Property code	Value	Unit	Source
hf	-642.40	kJ/mol	Cheméo Relay (1.0)
hfus	37.94	kJ/mol	Joback Method
hvap	78.13	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.16		Cheméo Relay (1.0)
logp	5.273		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	1820.30		NIST Webbook
rinpol	1819.00		NIST Webbook
rinpol	1820.30		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1819.00		NIST Webbook
rinpol	1796.00		NIST Webbook
tb	570.61	K	Cheméo Relay (1.0)
tc	736.75	K	Cheméo Relay (1.0)
tf	227.40	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.05	J/mol×K	668.25	Joback Method
cpg	729.41	J/mol×K	697.65	Joback Method
cpg	746.91	J/mol×K	727.05	Joback Method
cpg	763.59	J/mol×K	756.46	Joback Method
cpg	779.47	J/mol×K	785.86	Joback Method
cpg	794.58	J/mol×K	815.26	Joback Method

cpg	808.95	J/mol×K	844.66	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72934179&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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