(Z)-Heptacos-18-ene-2,4-dione

Inchi: InChI=1S/C27H50O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-2
InchiKey: JOPYJNRQQOWTHX-KHPPLWFESA-N
Formula: C27H50O2
SMILES: CCCCCCCCC=CCCCCCCCCCCCCCC(=O)CC(C)=O
Mol. weight [g/mol]: 406.68
CAS: 305805-38-3

Physical Properties

Property code	Value	Unit	Source
gf	-1.16	kJ/mol	Joback Method
hf	-708.55	kJ/mol	Joback Method
hfus	69.09	kJ/mol	Joback Method
hvap	89.15	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.913		Crippen Method
mcvol	390.130	ml/mol	McGowan Method
pc	758.07	kPa	Joback Method
rinpol	3021.20		NIST Webbook
rinpol	3021.20		NIST Webbook
tb	929.06	K	Joback Method
tc	1140.18	K	Joback Method
tf	488.83	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1316.92	J/mol×K	929.06	Joback Method
cpg	1338.80	J/mol×K	964.25	Joback Method
cpg	1359.42	J/mol×K	999.43	Joback Method
cpg	1378.86	J/mol×K	1034.62	Joback Method
cpg	1397.22	J/mol×K	1069.81	Joback Method
cpg	1414.59	J/mol×K	1104.99	Joback Method
cpg	1431.04	J/mol×K	1140.18	Joback Method

dvisc	0.0007463	Pa×s	488.83	Joback Method
dvisc	0.0003075	Pa×s	562.20	Joback Method
dvisc	0.0001555	Pa×s	635.57	Joback Method
dvisc	0.0000905	Pa×s	708.94	Joback Method
dvisc	0.0000583	Pa×s	782.32	Joback Method
dvisc	0.0000405	Pa×s	855.69	Joback Method
dvisc	0.0000298	Pa×s	929.06	Joback Method

Sources

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=C305805383&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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