(Z)-Pentacos-16-ene-2,4-dione

Inchi: InChI=1S/C25H46O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25(27)2
InchiKey: MDFRVEWZNNVTRI-KHPPLWFESA-N
Formula: C25H46O2
SMILES: CCCCCCCCC=CCCCCCCCCCCCCC(=O)CC(C)=O
Mol. weight [g/mol]: 378.63
CAS: 305805-39-4

Physical Properties

Property code	Value	Unit	Source
gf	-18.00	kJ/mol	Joback Method
hf	-667.27	kJ/mol	Joback Method
hfus	63.91	kJ/mol	Joback Method
hvap	84.69	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	8.133		Crippen Method
mcvol	361.950	ml/mol	McGowan Method
pc	845.05	kPa	Joback Method
rinpol	2798.10		NIST Webbook
rinpol	2798.10		NIST Webbook
tb	883.30	K	Joback Method
tc	1081.46	K	Joback Method
tf	466.29	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.91	J/mol×K	883.30	Joback Method
cpg	1209.44	J/mol×K	916.33	Joback Method
cpg	1228.84	J/mol×K	949.35	Joback Method
cpg	1247.18	J/mol×K	982.38	Joback Method
cpg	1264.54	J/mol×K	1015.41	Joback Method
cpg	1280.98	J/mol×K	1048.44	Joback Method
cpg	1296.57	J/mol×K	1081.46	Joback Method

dvisc	0.0009593	Pa×s	466.29	Joback Method
dvisc	0.0004013	Pa×s	535.79	Joback Method
dvisc	0.0002050	Pa×s	605.29	Joback Method
dvisc	0.0001203	Pa×s	674.79	Joback Method
dvisc	0.0000780	Pa×s	744.30	Joback Method
dvisc	0.0000544	Pa×s	813.80	Joback Method
dvisc	0.0000402	Pa×s	883.30	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=C305805394&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