Heptacosane-6,8-dione

Inchi: InChI=1S/C27H52O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22-24-27(29)25-2
InchiKey: ZWDFZBUKKXMZLB-UHFFFAOYSA-N
Formula: C27H52O2
SMILES: CCCCCCCCCCCCCCCCCCCC(=O)CC(=O)CCCCC
Mol. weight [g/mol]: 408.70

Physical Properties

Property code	Value	Unit	Source
gf	-81.38	kJ/mol	Joback Method
hf	-825.77	kJ/mol	Joback Method
hfus	68.88	kJ/mol	Joback Method
hvap	89.19	kJ/mol	Joback Method
log10ws	-9.68		Crippen Method
logp	9.137		Crippen Method
mcvol	394.430	ml/mol	McGowan Method
pc	736.82	kPa	Joback Method
rinpol	2988.40		NIST Webbook
rinpol	2988.40		NIST Webbook
tb	924.90	K	Joback Method
tc	1136.76	K	Joback Method
tf	493.91	K	Joback Method
vc	1.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.12	J/mol×K	924.90	Joback Method
cpg	1443.36	J/mol×K	1101.45	Joback Method
cpg	1426.03	J/mol×K	1066.14	Joback Method
cpg	1407.51	J/mol×K	1030.83	Joback Method
cpg	1387.74	J/mol×K	995.52	Joback Method
cpg	1366.64	J/mol×K	960.21	Joback Method
cpg	1459.59	J/mol×K	1136.76	Joback Method
dvisc	0.0000341	Pa×s	924.90	Joback Method

dvisc	0.0000462	Pa×s	853.07	Joback Method
dvisc	0.0000662	Pa×s	781.24	Joback Method
dvisc	0.0001022	Pa×s	709.40	Joback Method
dvisc	0.0001739	Pa×s	637.57	Joback Method
dvisc	0.0003384	Pa×s	565.74	Joback Method
dvisc	0.0007997	Pa×s	493.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U413392&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
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