

Tritriacontane-6.8-dione

Inchi: InChI=1S/C33H64O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32-33
InchiKey: VOJQUEYIAVHRFR-UHFFFAOYSA-N
Formula: C33H64O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)CC(=O)CCCCC
Mol. weight [g/mol]: 492.86

Physical Properties

Property code	Value	Unit	Source
gf	-30.86	kJ/mol	Joback Method
hf	-949.61	kJ/mol	Joback Method
hfus	84.42	kJ/mol	Joback Method
hvap	102.54	kJ/mol	Joback Method
log10ws	-12.20		Crippen Method
logp	11.477		Crippen Method
mvol	478.970	ml/mol	McGowan Method
pc	551.04	kPa	Joback Method
rinpol	3609.70		NIST Webbook
rinpol	3609.70		NIST Webbook
tb	1062.18	K	Joback Method
tc	1347.99	K	Joback Method
tf	561.53	K	Joback Method
vc	1.895	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1741.31	J/molxK	1062.18	Joback Method
cpg	1770.02	J/molxK	1109.81	Joback Method
cpg	1796.35	J/molxK	1157.45	Joback Method
cpg	1820.53	J/molxK	1205.08	Joback Method
cpg	1842.81	J/molxK	1252.72	Joback Method
cpg	1863.42	J/molxK	1300.35	Joback Method
cpg	1882.60	J/molxK	1347.99	Joback Method
dvisc	0.0003536	Paxs	561.53	Joback Method

dvisc	0.0001436	Paxs	644.97	Joback Method
dvisc	0.0000717	Paxs	728.41	Joback Method
dvisc	0.0000413	Paxs	811.85	Joback Method
dvisc	0.0000264	Paxs	895.30	Joback Method
dvisc	0.0000182	Paxs	978.74	Joback Method
dvisc	0.0000133	Paxs	1062.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414921&Units=SI

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

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