

Nonacosane-2,4-dione

Inchi: InChI=1S/C29H56O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29
InchiKey: MEQWKVIDALQQBU-UHFFFAOYSA-N
Formula: C29H56O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)CC(C)=O
Mol. weight [g/mol]: 436.75

Physical Properties

Property code	Value	Unit	Source
gf	-64.54	kJ/mol	Joback Method
hf	-867.05	kJ/mol	Joback Method
hfus	74.06	kJ/mol	Joback Method
hvap	93.64	kJ/mol	Joback Method
log10ws	-10.52		Crippen Method
logp	9.917		Crippen Method
mvol	422.610	ml/mol	McGowan Method
pc	665.63	kPa	Joback Method
rinpol	3242.10		NIST Webbook
rinpol	3242.10		NIST Webbook
tb	970.66	K	Joback Method
tc	1201.41	K	Joback Method
tf	516.45	K	Joback Method
vc	1.671	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.89	J/molxK	970.66	Joback Method
cpg	1499.09	J/molxK	1009.12	Joback Method
cpg	1521.63	J/molxK	1047.58	Joback Method
cpg	1542.62	J/molxK	1086.04	Joback Method
cpg	1562.17	J/molxK	1124.49	Joback Method
cpg	1580.39	J/molxK	1162.95	Joback Method
cpg	1597.38	J/molxK	1201.41	Joback Method
dvisc	0.0006151	Paxs	516.45	Joback Method

dvisc	0.0002565	Paxs	592.15	Joback Method
dvisc	0.0001304	Paxs	667.85	Joback Method
dvisc	0.0000761	Paxs	743.56	Joback Method
dvisc	0.0000491	Paxs	819.26	Joback Method
dvisc	0.0000341	Paxs	894.96	Joback Method
dvisc	0.0000250	Paxs	970.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412903&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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