Tricosane-4,6-dione

Inchi: InChI=1S/C23H44O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20-23(25)21-22(24)19
InchiKey: OSWNBDSFXXEWTJ-UHFFFAOYSA-N
Formula: C23H44O2
SMILES: CCCCCCCCCCCCCCCCCC(=O)CC(=O)CCC
Mol. weight [g/mol]: 352.59
CAS: 289681-93-2

Physical Properties

Property code	Value	Unit	Source
gf	-115.06	kJ/mol	Joback Method
hf	-743.21	kJ/mol	Joback Method
hfus	58.52	kJ/mol	Joback Method
hvap	80.28	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	7.576		Crippen Method
mcvol	338.070	ml/mol	McGowan Method
pc	918.27	kPa	Joback Method
rinpol	2583.70		NIST Webbook
rinpol	2583.70		NIST Webbook
tb	833.38	K	Joback Method
tc	1020.75	K	Joback Method
tf	448.83	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.15	J/mol×K	833.38	Joback Method
cpg	1109.17	J/mol×K	864.61	Joback Method
cpg	1128.09	J/mol×K	895.84	Joback Method
cpg	1145.98	J/mol×K	927.07	Joback Method
cpg	1162.87	J/mol×K	958.29	Joback Method
cpg	1178.82	J/mol×K	989.52	Joback Method
cpg	1193.85	J/mol×K	1020.75	Joback Method

dvisc	0.0013047	Pa×s	448.83	Joback Method
dvisc	0.0005709	Pa×s	512.92	Joback Method
dvisc	0.0003002	Pa×s	577.01	Joback Method
dvisc	0.0001795	Pa×s	641.11	Joback Method
dvisc	0.0001178	Pa×s	705.20	Joback Method
dvisc	0.0000830	Pa×s	769.29	Joback Method
dvisc	0.0000617	Pa×s	833.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C289681932&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

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