

Tricosane-6,8-dione

Inchi:	InChI=1S/C23H44O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-18-20-23(25)21-22(24)19-17-6
InchiKey:	XKMZZUYCBHPSGA-UHFFFAOYSA-N
Formula:	C23H44O2
SMILES:	CCCCCCCCCCCCCCCC(=O)CC(=O)CCCC
Mol. weight [g/mol]:	352.59
CAS:	95605-23-5

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
mvol	338.070	ml/mol	McGowan Method
pc	918.27	kPa	Joback Method
rinpol	2576.30		NIST Webbook
rinpol	2576.30		NIST Webbook
tb	833.38	K	Joback Method
tc	1020.75	K	Joback Method
tf	448.83	K	Joback Method
vc	1.335	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C95605235&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
mvol:	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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