

Icosane-6,8-dione

Inchi:	InChI=1S/C20H38O2/c1-3-5-7-8-9-10-11-12-13-15-17-20(22)18-19(21)16-14-6-4-2/h3-18
InchiKey:	RPQVHNSWIOVYEA-UHFFFAOYSA-N
Formula:	C20H38O2
SMILES:	CCCCCCCCCCCC(=O)CC(=O)CCCCC
Mol. weight [g/mol]:	310.51

Physical Properties

Property code	Value	Unit	Source
gf	-140.32	kJ/mol	Joback Method
hf	-681.29	kJ/mol	Joback Method
hfus	50.75	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	6.406		Crippen Method
mcvol	295.800	ml/mol	McGowan Method
pc	1102.28	kPa	Joback Method
rinpol	2274.00		NIST Webbook
rinpol	2274.00		NIST Webbook
tb	764.74	K	Joback Method
tc	942.91	K	Joback Method
tf	415.02	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.39	J/molxK	764.74	Joback Method
cpg	924.02	J/molxK	794.43	Joback Method
cpg	941.72	J/molxK	824.13	Joback Method
cpg	958.52	J/molxK	853.82	Joback Method
cpg	974.45	J/molxK	883.52	Joback Method
cpg	989.55	J/molxK	913.21	Joback Method
cpg	1003.84	J/molxK	942.91	Joback Method
dvisc	0.0018113	Paxs	415.02	Joback Method

dvisc	0.0008163	Paxs	473.31	Joback Method
dvisc	0.0004381	Paxs	531.59	Joback Method
dvisc	0.0002659	Paxs	589.88	Joback Method
dvisc	0.0001766	Paxs	648.17	Joback Method
dvisc	0.0001254	Paxs	706.45	Joback Method
dvisc	0.0000939	Paxs	764.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U413682&Units=SI
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

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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