GA73, Me

Other names: GA73, Methyl ester
Inchi: InChI=1S/C20H24O4/c1-11-9-19-10-12(11)5-6-13(19)20-8-4-7-18(2,17(22)24-20)15(20)1
InchiKey: HQSDLFRIZKDOEE-SRYNXPEOSA-N
Formula: C20H24O4
SMILES: C=C1CC23CC1CC=C2C12CCCC(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 328.40

Physical Properties

Property code	Value	Unit	Source
gf	3.67	kJ/mol	Joback Method
hf	-463.02	kJ/mol	Joback Method
hfus	26.16	kJ/mol	Joback Method
hvap	75.29	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.174		Crippen Method
mcvol	244.640	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	2344.00		NIST Webbook
rinpol	2326.00		NIST Webbook
rinpol	2344.00		NIST Webbook
rinpol	2329.00		NIST Webbook
rinpol	2326.00		NIST Webbook
rinpol	2325.00		NIST Webbook
tb	869.65	K	Joback Method
tc	1121.85	K	Joback Method
tf	659.19	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.47	J/mol×K	869.65	Joback Method
cpg	879.99	J/mol×K	911.68	Joback Method
cpg	908.21	J/mol×K	953.72	Joback Method

cpg	938.73	J/mol×K	995.75	Joback Method
cpg	972.10	J/mol×K	1037.79	Joback Method
cpg	1008.92	J/mol×K	1079.82	Joback Method
cpg	1049.75	J/mol×K	1121.85	Joback Method

Sources

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=R79896&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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