GA73 Methyl ester, [D2]

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-SUTRIPOASA-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	2328.00		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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R499877&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
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