3-(3-Methoxy-4-cyclohexylmethoxy-phenyl)-2-met
acid, methyl ester

Inchi: InChI=1S/C19H28O4/c1-14(19(20)22-3)11-16-9-10-17(18(12-16)21-2)23-13-15-7-5-4-6-8
InchiKey: MTLSNKDBKZHSKU-UHFFFAOYSA-N
Formula: C19H28O4
SMILES: COC(=O)C(C)Cc1ccc(OCC2CCCCC2)c(OC)c1
Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-219.66	kJ/mol	Joback Method
hf	-682.10	kJ/mol	Joback Method
hfus	31.70	kJ/mol	Joback Method
hvap	75.50	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.006		Crippen Method
mcvol	263.130	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	2272.10		NIST Webbook
rinpol	2272.10		NIST Webbook
tb	811.00	K	Joback Method
tc	1028.38	K	Joback Method
tf	464.35	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.15	J/mol×K	811.00	Joback Method
cpg	902.53	J/mol×K	992.15	Joback Method
cpg	889.83	J/mol×K	955.92	Joback Method
cpg	875.65	J/mol×K	919.69	Joback Method
cpg	859.98	J/mol×K	883.46	Joback Method
cpg	842.82	J/mol×K	847.23	Joback Method
cpg	913.75	J/mol×K	1028.38	Joback Method
dvisc	0.0000473	Pa×s	811.00	Joback Method

dvisc	0.0000617	Pa×s	753.22	Joback Method
dvisc	0.0000841	Pa×s	695.45	Joback Method
dvisc	0.0001211	Pa×s	637.67	Joback Method
dvisc	0.0001877	Pa×s	579.90	Joback Method
dvisc	0.0003206	Pa×s	522.12	Joback Method
dvisc	0.0006256	Pa×s	464.35	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=R157885&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
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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