

(4-cyclohexylmethoxy-phenyl)-acetic acid, methyl ester

Inchi:	InChI=1S/C16H22O3/c1-18-16(17)11-13-7-9-15(10-8-13)19-12-14-5-3-2-4-6-14/h7-10,14
InchiKey:	POIWXNWRDGTRTM-UHFFFAOYSA-N
Formula:	C16H22O3
SMILES:	COC(=O)Cc1ccc(OCC2CCCCC2)cc1
Mol. weight [g/mol]:	262.34

Physical Properties

Property code	Value	Unit	Source
gf	-127.85	kJ/mol	Joback Method
hf	-471.21	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	66.14	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.361		Crippen Method
mvol	214.990	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	2059.10		NIST Webbook
rinpol	2059.10		NIST Webbook
tb	715.40	K	Joback Method
tc	939.59	K	Joback Method
tf	410.79	K	Joback Method
vc	0.798	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.21	J/molxK	715.40	Joback Method
cpg	704.31	J/molxK	902.23	Joback Method
cpg	690.55	J/molxK	864.86	Joback Method
cpg	675.48	J/molxK	827.50	Joback Method
cpg	659.08	J/molxK	790.13	Joback Method
cpg	641.33	J/molxK	752.77	Joback Method
cpg	716.79	J/molxK	939.59	Joback Method
dvisc	0.0000990	Paxs	715.40	Joback Method

dvisc	0.0001281	Paxs	664.63	Joback Method
dvisc	0.0001730	Paxs	613.86	Joback Method
dvisc	0.0002466	Paxs	563.10	Joback Method
dvisc	0.0003771	Paxs	512.33	Joback Method
dvisc	0.0006332	Paxs	461.56	Joback Method
dvisc	0.0012086	Paxs	410.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R158071&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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