

3-(4-cyclohexyl-methyl-oxy-phenyl)-propionic acid, methyl ester

Inchi:	InChI=1S/C17H24O3/c1-19-17(18)12-9-14-7-10-16(11-8-14)20-13-15-5-3-2-4-6-15/h7-8,
InchiKey:	LJASMOYSLUNUSB-UHFFFAOYSA-N
Formula:	C17H24O3
SMILES:	COC(=O)CCc1ccc(OCC2CCCCC2)cc1
Mol. weight [g/mol]:	276.37

Physical Properties

Property code	Value	Unit	Source
gf	-119.43	kJ/mol	Joback Method
hf	-491.85	kJ/mol	Joback Method
hfus	29.25	kJ/mol	Joback Method
hvap	68.37	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.751		Crippen Method
mcvol	229.080	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	2158.60		NIST Webbook
tb	738.28	K	Joback Method
tc	958.89	K	Joback Method
tf	422.06	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.45	J/molxK	738.28	Joback Method
cpg	697.66	J/molxK	775.05	Joback Method
cpg	715.48	J/molxK	811.82	Joback Method
cpg	731.95	J/molxK	848.58	Joback Method
cpg	747.07	J/molxK	885.35	Joback Method
cpg	760.88	J/molxK	922.12	Joback Method
cpg	773.40	J/molxK	958.89	Joback Method
dvisc	0.0011148	Paxs	422.06	Joback Method
dvisc	0.0005764	Paxs	474.76	Joback Method

dvisc	0.0003400	Paxs	527.47	Joback Method
dvisc	0.0002208	Paxs	580.17	Joback Method
dvisc	0.0001540	Paxs	632.87	Joback Method
dvisc	0.0001136	Paxs	685.58	Joback Method
dvisc	0.0000875	Paxs	738.28	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=R157929&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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