3-(4-Tolyl)butanoic acid methyl ester

Inchi: InChI=1S/C12H16O2/c1-9-4-6-11(7-5-9)10(2)8-12(13)14-3/h4-7,10H,8H2,1-3H3
InchiKey: OBWVAZIGRGXGIB-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: COC(=O)CC(C)c1ccc(C)cc1
Mol. weight [g/mol]: 192.25
CAS: 24254-66-8

Physical Properties

Property code	Value	Unit	Source
gf	-83.42	kJ/mol	Joback Method
hf	-316.03	kJ/mol	Joback Method
hfus	19.75	kJ/mol	Joback Method
hvap	54.01	kJ/mol	Joback Method
ie	8.20 ± 0.20	eV	NIST Webbook
log10ws	-2.83		Crippen Method
logp	2.662		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
tb	581.47	K	Joback Method
tc	792.78	K	Joback Method
tf	321.10	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.16	J/mol×K	581.47	Joback Method
cpg	462.32	J/mol×K	757.56	Joback Method
cpg	450.30	J/mol×K	722.34	Joback Method
cpg	437.50	J/mol×K	687.12	Joback Method
cpg	423.89	J/mol×K	651.91	Joback Method
cpg	409.45	J/mol×K	616.69	Joback Method
cpg	473.55	J/mol×K	792.78	Joback Method
dvisc	0.0001687	Pa×s	581.47	Joback Method

dvisc	0.0002174	Pa×s	538.08	Joback Method
dvisc	0.0002929	Pa×s	494.68	Joback Method
dvisc	0.0004180	Pa×s	451.29	Joback Method
dvisc	0.0006432	Pa×s	407.89	Joback Method
dvisc	0.0010969	Pa×s	364.50	Joback Method
dvisc	0.0021607	Pa×s	321.10	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24254668&Units=SI

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/39-828-0/3-4-Tolyl-butanoic-acid-methyl-ester.pdf
Generated by Cheméo on 2025-12-23 06:06:16.900978959 +0000 UTC m=+6218174.431019612.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.