

Malonic acid, butyl 3-heptyl ester

Inchi:	InChI=1S/C14H26O4/c1-4-7-9-12(6-3)18-14(16)11-13(15)17-10-8-5-2/h12H,4-11H2,1-3H
InchiKey:	RMUNWABFGYIVNJ-UHFFFAOYSA-N
Formula:	C14H26O4
SMILES:	CCCCOC(=O)CC(=O)OC(CC)CCCC
Mol. weight [g/mol]:	258.35

Physical Properties

Property code	Value	Unit	Source
gf	-403.28	kJ/mol	Joback Method
hf	-827.17	kJ/mol	Joback Method
hfus	34.07	kJ/mol	Joback Method
hvap	64.68	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.232		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
tb	671.86	K	Joback Method
tc	850.20	K	Joback Method
tf	376.86	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.64	J/molxK	671.86	Joback Method
cpg	694.61	J/molxK	820.48	Joback Method
cpg	681.70	J/molxK	790.75	Joback Method
cpg	668.05	J/molxK	761.03	Joback Method
cpg	653.66	J/molxK	731.31	Joback Method
cpg	638.53	J/molxK	701.58	Joback Method
cpg	706.79	J/molxK	850.20	Joback Method
dvisc	0.0001111	Paxs	671.86	Joback Method

dvisc	0.0001474	Paxs	622.69	Joback Method
dvisc	0.0002052	Paxs	573.53	Joback Method
dvisc	0.0003039	Paxs	524.36	Joback Method
dvisc	0.0004883	Paxs	475.19	Joback Method
dvisc	0.0008752	Paxs	426.03	Joback Method
dvisc	0.0018269	Paxs	376.86	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U349149&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
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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