

Fumaric acid, dodecyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C21H38O4/c1-5-6-7-8-9-10-11-12-13-14-17-24-20(22)15-16-21(23)25-19(4)18
InchiKey: UVAPLAFAYKQROY-FOCLMDBBSA-N
Formula: C21H38O4
SMILES: CCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-266.56	kJ/mol	Joback Method
hf	-859.71	kJ/mol	Joback Method
hfus	48.88	kJ/mol	Joback Method
hvap	79.83	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.594		Crippen Method
mvol	317.330	ml/mol	McGowan Method
pc	1058.26	kPa	Joback Method
rinpol	2375.00		NIST Webbook
rinpol	2375.00		NIST Webbook
tb	835.74	K	Joback Method
tc	1026.32	K	Joback Method
tf	435.67	K	Joback Method
vc	1.228	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.42	J/molxK	835.74	Joback Method
cpg	1023.65	J/molxK	867.50	Joback Method
cpg	1040.79	J/molxK	899.27	Joback Method
cpg	1056.86	J/molxK	931.03	Joback Method
cpg	1071.91	J/molxK	962.79	Joback Method
cpg	1085.96	J/molxK	994.56	Joback Method
cpg	1099.04	J/molxK	1026.32	Joback Method
dvisc	0.0009905	Paxs	435.67	Joback Method

dvisc	0.0003880	Paxs	502.35	Joback Method
dvisc	0.0001893	Paxs	569.03	Joback Method
dvisc	0.0001074	Paxs	635.70	Joback Method
dvisc	0.0000678	Paxs	702.38	Joback Method
dvisc	0.0000464	Paxs	769.06	Joback Method
dvisc	0.0000337	Paxs	835.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348084&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

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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