Fumaric acid, dodecyl 3-methylbut-3-enyl ester

Inchi: InChI=1S/C21H36O4/c1-4-5-6-7-8-9-10-11-12-13-17-24-20(22)14-15-21(23)25-18-16-19

InchiKey: DTCZUGWZQZXGMM-CCEZHUSRSA-N

Formula: C21H36O4

SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCCCCCCCCCCC

Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-182.39	kJ/mol	Joback Method
hf	-733.51	kJ/mol	Joback Method
hfus	53.33	kJ/mol	Joback Method
hvap	80.02	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.516		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1079.93	kPa	Joback Method
rinpol	2465.00		NIST Webbook
rinpol	2465.00		NIST Webbook
tb	833.18	K	Joback Method
tc	1023.20	K	Joback Method
tf	449.95	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.61	J/mol×K	833.18	Joback Method
cpg	994.23	J/mol×K	864.85	Joback Method
cpg	1010.84	J/mol×K	896.52	Joback Method
cpg	1026.46	J/mol×K	928.19	Joback Method
cpg	1041.13	J/mol×K	959.86	Joback Method
cpg	1054.89	J/mol×K	991.53	Joback Method
cpg	1067.76	J/mol×K	1023.20	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=U348911&Units=SI

Legend

cpg:	Ideal gas heat capacity
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