

Fumaric acid, naphth-1-yl 3-methylbut-2-yl ester

Inchi:	InChI=1S/C19H20O4/c1-13(2)14(3)22-18(20)11-12-19(21)23-17-10-6-8-15-7-4-5-9-16(15)
InchiKey:	OZRJZSNTASXVQU-VAWYXSNFSA-N
Formula:	C19H20O4
SMILES:	CC(C)C(C)OC(=O)C=CC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]:	312.36

Physical Properties

Property code	Value	Unit	Source
gf	-73.97	kJ/mol	Joback Method
hf	-402.30	kJ/mol	Joback Method
hfus	34.37	kJ/mol	Joback Method
hvap	79.96	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	3.889		Crippen Method
mcvol	245.930	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	2419.00		NIST Webbook
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tb	840.62	K	Joback Method
tc	1067.69	K	Joback Method
tf	484.77	K	Joback Method
vc	0.929	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.87	J/molxK	840.62	Joback Method
cpg	734.06	J/molxK	878.47	Joback Method
cpg	747.18	J/molxK	916.31	Joback Method
cpg	759.30	J/molxK	954.16	Joback Method
cpg	770.49	J/molxK	992.00	Joback Method
cpg	780.81	J/molxK	1029.85	Joback Method
cpg	790.35	J/molxK	1067.69	Joback Method
dvisc	0.0008518	Paxs	484.77	Joback Method

dvisc	0.0004777	Paxs	544.08	Joback Method
dvisc	0.0003001	Paxs	603.39	Joback Method
dvisc	0.0002049	Paxs	662.69	Joback Method
dvisc	0.0001490	Paxs	722.00	Joback Method
dvisc	0.0001137	Paxs	781.31	Joback Method
dvisc	0.0000901	Paxs	840.62	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=U405805&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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